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FLUME COMPUTER-AIDED DESIGN (CAD): INTEGRATED CAD FOR MICROFLUME COMPONENTS AND SYSTEMS

Microcosm Technologies, Incorporated

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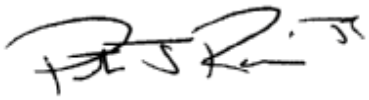
APPROVED: 

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13. ABSTRACT ***(Maximum 200 Words)***
This effort was aimed at developing a computer-aided design (CAD) system to allow start-to-finish design of a broad class of micromechanical fluid systems. The NetFlow program, previously completed under DARPA funding, developed the capability to model the diverse transport phenomena that are present in micromechanical systems. FlumeCAD extends this toolkit to include simulation of active components as well as providing the capability to extract behavior models. Tools for simulating the entire device at the full time domain system level were also developed. All original milestones were met and the FlumeCAD software has been successfully released commercially.

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Research Overview

This report serves as the final summary of our research under the FlumeCAD program as part of the Composite CAD Program. In this report we will discuss the proposed objectives of the FlumeCAD program and the accomplishments over the course of the program.

Program Summary

The goal of the FlumeCAD project is to create a CAD system to allow start-to-finish design of a broad class of Microchemical Fluidic Systems. This requires the capability for full simulation of the microfluidic molecular system (Microflume) systems at a time domain system level and tools for optimizing and programming designs. Typical microchemical systems comprise of both active and passive components. Examples of active components include switches, injectors, reaction wells etc. Passive components, on the other hand, are the wires connecting the active components to create the entire device. At Coventor, we have undertaken the task of providing the design capability for the entire system. The first part of this program was the NetFlow project, previously completed under DARPA funding. The NetFlow program was aimed at developing the capability to model the diverse transport phenomena that are present in microchemical systems – these include pressure driven, electrokinetic and diffusive transport. The FlumeCAD program extends this toolkit to include the simulation of the active components as well as provide the capability to extract behavioral models for the individual components. Tools for simulating the entire device at the full time domain system level are also part of this program.

The overall program summary is as follows:

- All milestones originally set forth in the program have been met. Some of the tasks were completed well ahead of schedule, whereas some others were delayed for various reasons, but we were able to accommodate the delays by faster progress in other areas.

- The FlumeCAD software has been released commercially. Four versions of the software were released during the course of this program – each version added new functionality and enhanced existing functionality based on user feedback and program milestones. Additionally a newer version has been released in Q1 2001, after the completion of the program. Future releases are planned in the next several years. The software is available on Sun, HP, SGI and Windows NT Platforms. The User's Guide and Reference Manuals give much more details about the software and its use.

- The FlumeCAD tool set allows start-to-finish design of the entire microchemical device. This includes:
    - Enhancements to the layout generator to support fluidic devices. This includes support for curves, layout generators for characteristic geometries relevant to microchemical devices and interoperability with a wide variety of standards.
    - Mesh Generation for isotropically etched cross sections as is typical of these devices. Additionally mesh generation for circular and trapezoidal cross sections is also supported at FlumeCAD user request.
    - A set of solvers for active component modeling including switching, injection, reactions etc. Passive component modeling is also incorporated within the FlumeCAD suite and was developed under NetFlow.
    - FlowMM, an extraction tool for extracting behavioral models for flow resistance and inertance through microchannels. This is since been expanded to other models as well.

    - FlowLib, a library of parameterized components for time-domain system simulation of microchemical devices. This includes transport components, mechanical actuators, electrokinetic injection and switching components as well as several other components relevant to typical devices.
- The software tools are in continued development with additional releases planned for the next several years. Current users include both industrial and academic groups.
- Experimental support for the program was provided by Caliper Technologies and the University of Washington. Caliper provided Coventor with data from electrokinetic experiments, including switching, dispensing, converters and reaction experiments. UW provided Coventor with data from the no-moving-parts valve driven pump and shared data about an H-filter from an associated group. In addition, Coventor obtained validation data from Harvard, Gamera Biosciences, Berkeley, Stanford and several other groups to assist in our development.
- FlumeCAD has been applied in predictive design of electrokinetic components that have subsequently been validated experimentally. In each case, the component behavior was significantly enhanced after the CAD design. To our knowledge, this is the first example of the successful application of CAD tools in this area.
- Data analysis tools were developed in the program to enable the validation of simulation and experimental results. These tools are available as part of the software.
- Several research publications and presentations have emerged over the course of this program. This includes papers at μTAS, Hilton Head and MEMS. A complete list including copies of papers is attached in Appendix 1.
- FlumeCAD use in component and system design was referenced in 13 papers at μTAS 2000.

Section 1: Introduction

Overview

The libraries have been developed to allow system level designers to incorporate MEMS (Micro Electrical Mechanical Systems) into their design using a top-down system level approach. Use of the models supplied with these libraries enables system designers to simulate and rapidly evaluate multiple options and feed highly accurate behavioral models to the device designer. The behavioral models describe building blocks for a MEMS device. A designer using the behavioral models need not start from scratch by designing and modeling every element of the MEMS device. The use of these models provides a top-down method to design a MEMS device much faster and more reliably than using a bottom-up detailed device model and analysis. For example, the results of a benchmark design effort comparing the time required for a top-down design with the time required for a bottom-up design showed a time savings of nearly 4 weeks for the same device. Depending on the complexity of the design, the time savings could be even greater. Furthermore, the number of prototyping cycles needed to complete the product design could be reduced, as the system model analyzes a much more detailed, complex behavior than even the most extensive FEM analysis could. Finally, in addition to productivity gains resulting from the time savings, the top-down approach reduces personnel training requirements because system designers will not be required to be MEMS design experts. The following table shows the libraries available and their respective documentation.

Library	Document Title	Description	Section
Electromechanical	Behavioral Models for Electromechanical Simulation	Introduction	1
		Model Description	2
		Tutorial	3
Optics	Behavioral Models for Optical Simulation	Introduction	1
		Model Description and Examples	2
Fluidics	Behavioral Models for Microfluidics Simulation	Introduction	1
		Model Description	2
		Tutorial	3

1.1: Fluidics Model Library

The library consists of four channels (Straight Channel, Elbow, U-Bend, and a Right Angle channel), Meander, Reservoir, Diodic Valve, FlowMM resistor, Low Reynolds number Orifice, Piston, Meniscus, and ES (electrostatic) actuator. The ES actuator has a voltage as input and displacement as output. The Piston ports correspond to displacement and pressure difference. This allows the user to analyze networks of channels orders of magnitude faster than full 3-D simulation.

Section 2: Model Description

2.1: Overview

Modeling fluidic systems is analogous to modeling electrical circuits. In electrical circuits, current flows through an element when voltage is applied. For example, an electrical resistor performs according to Ohm's law: V = IR, where V is the voltage difference, I is the current, and R is the resistance. In this sense, we say that the "across" variable is voltage and the "through" variable is the flow rate. An example is a pipe in a home plumbing system that may have water flowing through it at some rate. The rate is determined by the pressure within the municipal water main. The pipe itself has some resistance (R), which can be determined with the formula P = QR where the pressure drop (P) and the flow rate (Q) are known. Fluid resistance is illustrated by the difference of effort required to drink a milk shake or water through a straw. In this example, the resistance to flow can be reduced when a straw with a larger diameter is used. The home plumbing system can be drawn as a network of fluid resistors with each having an R value determined by its diameter and curvature (or angle). Abstracting a three-dimensional home plumbing network as a circuit of resistors illustrates the basic concept of system modeling for fluidic networks.

A fluidic network can be composed of several different elements connected by wires. The wires represent a connection between the elements that communicates only the P and Q values. Each element behaves with a certain relationship between P and Q, and the system as a whole is solved so every wire between elements has a net flow in equal to the net flow out, which in electrical circuits is called Kirchoff's Law. For example, flow that enters the bottom of a T-junction can go out the top either to the left or the right. The sum of the flows through the arms must equal the flow entering the bottom. In system modeling, a connection of wires like this is referred to as a node. The solution to the system is found when all nodes have a sum of flows equal to zero. Basically, the system can be as complicated as desired, but in the end elements are only plugged into adjacent elements.

A great deal of experience in analyzing circuits has been gained by electrical circuit designers. Because of their analogous natures, the same principles can be directly applied to fluidic networks. Systems can be analyzed for steady state solutions (DC Operating Point), flows that change in time (Transient analysis), resonances (AC analysis), loops through a range of element properties and a host of other useful analyses. The analysis output is a graphical tool that shows signals versus time. Post-processing of the signals allows the user to seek whatever useful information is desired.

The greatest benefit of system modeling is the speed of a design cycle, where runs can be repeated for different element properties in mere seconds, compared to complete recalculation of a full three-dimensional problem that could take hours or days. Speed up is possible because the full three-dimensional behavior has been preprocessed and extracted, either analytically or empirically, and reduced to a non-linear relationship (usually an ordinary differential equation or ODE) between P and Q. It is for this reason that library elements are for specific geometries or physical cases and are tailored for the problems the user wants to solve.

The library elements provided by FlowLib include a variety of channels for pressure-driven flows, electrokinetic elements for studying electrokinetic transport of species such as DNA, meniscus elements for modeling a liquid-gas interface, some specialized elements for internal flows, and transducers for expanding the network to mechanical or electrical domains. The library includes a pair of elements to link up with the FlowMM module that extracts flow behavior of an arbitrary two-port element. The complete list of library elements is found in the table on the next page.

Internal Flow Models	Straight channel
	Elbow
	U-bend
	Right angled channel
	Meander
	Air pocket (linear and nonlinear)
	Burst valve
	Reservoir
	Diodic valve
	Low Reynolds number orifice
Meniscus Models	Spherical Droplet (1 or 2 port)
	Head/Neck Model of Droplet (1 or 2 port)
Actuators	Piston
	Parallel plate capacitor
	Edge-fixed membrane
	ES (electrostatic) actuator
Electrokinetic Elements	Electrokinetic channel – straight
	Electrokinetic channel – elbow
	Electrokinetic channel – u-bend
	Electrokinetic channel – two species straight
	Electrokinetic channel – two species elbow
	Electrokinetic channel – two species u-bend
	Electrokinetic injector
Flow MM Elements	FlowMM resistor
	FlowMM resistor and inertor

2.2: Library Description

2.2.1 Fluid Models

Each of the system model components of the MemSys fluidics library is discussed in detail in the next section. This includes a description of the model, the types of port(s) connected to the component, and the input required by the user. The "through" and "across" variables that characterize most of the components are as follows:

Hydraulic domain: Flow Rate, Pressure
Mechanical domain: Force, Displacement
Electrical domain: Current, Voltage

Some of the components will have a combination of hydraulic (pressure), mechanical (displacement), and electrical (voltage) ports. Note that this concept of the "through" and "across" variable does not apply to the electrokinetic elements. The units for the input variables are in MKS. In some cases default values are shown (e.g. mobility=20n). The table below describes the notation that may be used to set values in the input fields.

t	tera (10^{12})	u	micro (10^{-6})
g	giga (10^{9})	n	nano (10^{-9})
meg	mega (10^{6})	p	pico (10^{-12})
k	kilo (10^{3})	f	femto (10^{-15})
m	milli (10^{-3})	a	atto (10^{-18})

2.2.2 Cross Sections

Circular, rectangular, and D-shaped cross section dimensions are shown in Figure 2-1.

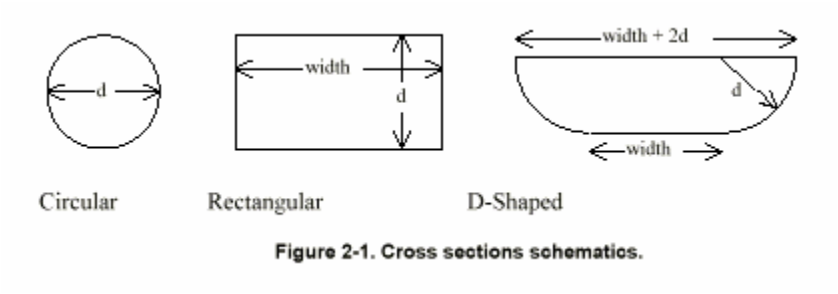


Figure 2-1. Cross sections schematics.

2.3: Model Descriptions

2.3.1 Air Pocket

This template models an air pocket as an ideal gas undergoing compression and expansion. The pin "x" is a translational pin representing the position of a piston that exerts a force against the gas. The other walls surrounding the gas are all fixed to ground. The equilibrium state of the gas is at pressure p_0 and volume height_0*area, and the gas has an adiabatic gas constant gamma (C_P/C_V), which for air is typically 1.4. The thermodynamic process governing the change of state of the gas is either adiabatic (insulated) or isothermal (temperature is constant). A polytropic process can be modeled by changing gamma to a value between 1 and 1.4. Note that the maximum positive force the air_pocket model simulates (when the air pocket is being expanded) is area*p_0, so expanding with a force more than that can result in an unstable regime.

Symbol Name: air_pocket

Port: x (mechanical)

User Input	Description
p_0=101300	equilibrium pressure (default is atmospheric)
height_0	equilibrium height of air pocket
area	area of air pocket
gamma=1.4	adiabatic gas constant (Cp/Cv=1.4 for air)
thermodynamics	adiabatic or isothermal

2.3.2 Air Pocket – Linearized

This template models an air pocket as an ideal gas undergoing compression and expansion. The force is linearized about the equilibrium position in this model and should not be used if the displacements are greater than 5% of the height.

Symbol Name: air_pocket_lin

Port: x (mechanical)

User Input	Description
p_0=101300	equilibrium pressure
height_0	equilibrium height of air pocket
area	area of air pocket
gamma=1.4	adiabatic gas constant (Cp/Cv=1.4 for air)
thermodynamics	adiabatic or isothermal

2.3.3 Burst Valve

This template represents a burst valve, or as it is sometimes known, a capillary break. Fluid in a circular channel reaches a square_edged opening into a larger channel, and a meniscus forms at the opening. The meniscus has a pressure drop associated with it that can prevent the fluid from exiting the channel, and therefore acts as a valve.

This model assumes the valve is used only once, and once it has burst, the valve acts as a low-Reynolds-number orifice. The valve does not form again if the flow reverses after bursting.

The model assumes the opening is circular and the edge is square; that is, the wall outside the opening is perpendicular to the inner surface of the opening. The burst pressure and burst volume are that of a meniscus shaped as a spherical section, where p = 2*surface_tension/radius. The valve bursts when the volume equals the burst volume. The default value for surface_tension is that of water at 15.6 degrees C.

The meniscus attaches to the corner of the opening, with an angle measured inside the fluid to a line parallel to the wall outside the opening of contact_angle degrees. A contact angle near zero corresponds to a highly wetting fluid, and a contact angle greater than ninety degrees would correspond to a non-wetting fluid.

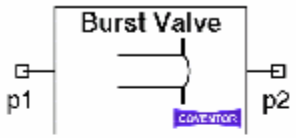
If the contact angle is greater than ninety degrees, the model will still determine the burst condition, but the shape of the meniscus at burst will be a spherical section larger than a hemisphere. The "burst_pressure" would be lower than the pressure of a hemisphere "max_pressure", but the pressure_drop signal might show a value higher than the burst_pressure, which, occurred when the meniscus was about the size of a hemisphere. The diameter of the inlet must be smaller than the diameter of the outlet.

The output signal "pressure_drop" shows the pressure drop the burst valve exerts on the system over time. The value changes suddenly upon bursting to that of a low-Reynolds-number orifice.

The event signal "counter" switches from zero to one when the valve has burst. The output signal "volume" is the time integral of "flow_rate", which tracks the total amount of flow since the beginning of the

simulation that has passed through the opening. The input parameter "fill_volume" represents volume that will be filled before the meniscus reaches the burst valve, if the fluid is not yet at the opening. The default is zero. The output signals "burst_pressure", "max_pressure", and "burst_volume" are the constants determined by the model and are output for ease of use for plotting in Scope.

Symbol Name: burst_valve



Ports: p1, p2 (hydraulic)

User Input	Description
contact_angle	contact angle in degrees between fluid and material on wall at outlet
fill_volume=0	volume to fill before reaching valve
d_inlet	diameter of p1 side, where burst occurs
d_outlet	diameter of p2 side, must be larger than d_inlet
surface_tension=73.4m	surface tension

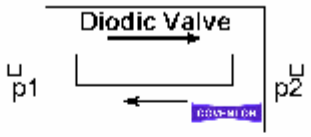
2.3.4 Diodic Valve

This template represents a generic flow channel with resistance and inertance, where the resistance depends on the direction of fluid flow. Therefore this can be used as a valve. Analogous to a diode in electrical circuits, this element is called a "diodic valve". Forward flow is defined as flow from p1 to p2.

The diodicity is a positive number denoting the ratio of the two flow rates measured when the same pressure difference is applied to the valve in forward and reverse directions. That is, if the flow rate is 20 in the forward direction, and 10 in the reverse direction, the diodicity is 2. The diodicity is assumed to be constant for all flow rates, so this is a linear diodic valve.

If flow_rate is positive, the resistance R is assumed to be that of a circular pipe, so the properties d, length, viscosity and density must be entered. If flow_rate is negative, the resistance is diodicity*R.

Symbol Name: diodic_valve



Ports: p1,p2 (hydraulic)

User Input	Description
d	Inner diameter of an equivalent circular pipe
length	Length of an equivalent circular pipe
viscosity	local viscosity
density	local density
diodicity	ratio of flow rates in and out of valve at same absolute pressure difference (default = 2)

2.3.5 Electrokinetic Elbow

This template models electrokinetic transport of a species along an elbow channel. The channel contains a medium in which the species has a diffusivity and a mobility. There is an electric field along the length of the channel, expressed in volts/meter. The species enters the channel as a band whose concentration versus distance is approximated as a gaussian distribution.

When connecting the electrostatic bend elements, use the right-handed (RH) or left-handed (LH) elements in the proper orientation. Do not flip these elements - only rotate them. Note that a right-handed element is different from a flipped left-handed element. If a bend element is flipped, it will not connect to the correct pins, and will result in errors in the output. Saber will not object to "height_out" being connected to "time_in".

The effect of the elbow is captured by a single parameter, alpha, where the full-width-half-maximum (fwhm) of a band after the bend is

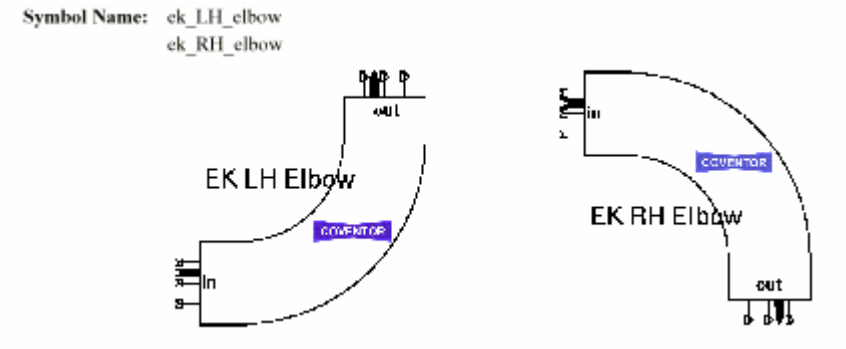
fwhm_exit = alpha + fwhm_s

where alpha is an additional width caused by distortion due to the bend, and fwhm_s is the full-width-half-maximum of the band after traversing a straight channel of equivalent length. The length of the path is the sum of two leg_lengths and one 90 degree bend of radius bend_radius.

The input pins denote the three quantities necessary to define the gaussian: height, width and time. The height is the
amplitude of the gaussian, the width is the full-width at half-maximum (fwhm) of the gaussian, and the time is the time when the gaussian enters the channel. The output pins denote the same quantities at the exit. Mobility, diffusivity and electric field are assumed to be constant along the channel.

DC operating point analysis of this model will generate the final state of the system: time the band enters and exits the channel, widths (fwhm, sigma, 1/e width) as the band enters and exits the channel, height as band enters and exits the channel, and velocity of the band. Tip: check the value of time_out of the last element in the channel to determine how long to run a transient analysis.

Transient analysis will produce quantities versus time, as the band resides in the channel. Signals are height, widths, and position. The concentration profile of the band in time is also output as band_input and band_output. To view band_input and band_output clearly, the timestep must be reduced to a value approximately 1e-6 to 1e-8 times the residence time. Use a large timestep during testing of the simulation until all desired settings are achieved. Then reduce the timestep until the gaussian bands become visible. The first run in transient analysis should have "End Time" set to the value of time_out of the last element in the channel. Using the calculator, the band_input and band_output could each be plotted versus position to show the concentration profile versus distance, rather than time. For example, select and place the two signals band_output and position into the calculator. Select Wave->f(x) and select "Graph X".



Input Ports	Description
height_in	height in
fwhm_in	Full-width-half_maximum in (meters)
time_in	time when band enters (s)

Output Ports	Description
height_out	height out
fwhm_out	full-width-half-maximum out (meters)
time_out	time when band reaches exit

User Input	Description
alpha = 0	Effective distortion of a bend due to the bend (alpha=0 is ideal)
leg_length = 0	Length of leg at each end of bend (m)
bend_radius = 1m	Radius of elbow (m)
electric_field = 10k	Electric field driving EK flow (V/m)
diffusivity = 5p	Diffusivity of the species in the medium (m^2/s)
mobility = 20n	Mobility of the species in the medium (m^2/Vs)

2.3.6 Electrokinetic Injector

This template represents an electrokinetic injector that outputs the width and height of a gaussian. The gaussian is the amplitude versus length taken from a detector located at the exit of the injector. The duration of the gaussian is taken to be the width at full-width-half-maximum. Full-width-half-maximum (fwhm) is the width of the gaussian at the height equal to half the maximum. The output height of the injector is the amplitude of the final gaussian band. The units are arbitrary, so are denoted "-".

The units of the output fwhm are meters. The functional form of the output fwhm is a fitted exponential with three parameters:

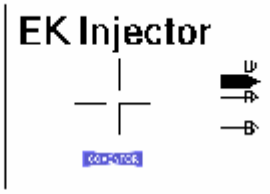
fwhm = velocity*coeff*exp(-1*x**exponent)

where coeff is the coefficient of a fitted exponential for the time the fwhm passes a detector. Multiplying by the velocity yields the width in meters of a band. The velocity is:

velocity = mobility*electric_field

where electric_field is the electric field in the exit arm of the injector.

Symbol Name: ek_injector



Output Ports	Description
height	height of band created by injector
fwhm	duration in seconds of band passing detection point measured at fwhm
time	time when peak of band exits injector

User Input	Description
x=30	Abscissa of fitted exponential
coeff=10	Coefficient of fitted exponential (s)
exponent=0.1	Exponent of fitted exponential
inj_height=1	Height of intensity pulse of injected band
inj_time=0	Time when injection begins (s)
electric_field = 10k	Electric field driving EK flow along exit arm (V/m)
mobility = 20n	Mobility of the species in the medium (m^2/Vs)

2.3.7 Electrokinetic Straight Channel

This template models electrokinetic transport of a species along a straight channel. The channel contains a medium in which the species has a diffusivity and a mobility. There is an electric field along the length of the channel, expressed in volts/meter. The species enters the channel as a band whose concentration versus distance is approximated as a gaussian distribution.

The input pins denote the three quantities necessary to define the gaussian: height, width, and time. The height is the amplitude of the gaussian, the width is the full-width at half-maximum (fwhm) of the gaussian, and the time is the time when the gaussian enters the channel. The output pins denote the same quantities at the exit.

Mobility, diffusivity, and electric field are assumed to be constant along the channel. DC operating point analysis of this model will generate the final state of the system: time the band enters and exits the channel, widths (fwhm, sigma, 1/e width) as the band enters and exits the channel, height as band enters and exits the channel, and velocity of the band. Tip: check the value of time_out of the last element in the channel so you have an idea of how long to run a transient analysis.

Transient analysis will produce quantities versus time, as the band resides in the channel. Signals are height, widths, and position. The concentration profile of the band in time is also output as band_input and band_output. To view band_input and band_output clearly, the timestep must be reduced to a value approximately 1e-6 to 1e-8 times the residence time. Use a large timestep during testing of the simulation until all desired settings are achieved. Then reduce the timestep until the gaussian bands become visible. The first run in transient analysis should have "End Time" set to the value of time_out of the last element in the channel.

Using the calculator, the band_input and band_output could each be plotted versus position to show the concentration profile versus distance, rather than time. For example, select and place the two signals band_output and position into the calculator. Select Wave->f(x) and select "Graph X".

Symbol Name: ek_straight

Input Ports	Description
height_in	height in
fwhm_in	full-width-half_maximum in (meters)
time_in	time when band enters (s)

Output Ports	Description
height_out	height out
fwhm_out	full-width-half-maximum out (meters)
time_out	time when band reaches exit

User Input	Description
channel_length = 50m	Length of separation channel (m)
electric_field = 10k	Electric field driving EK flow (V/m)
diffusivity = 5p	Diffusivity of the species in the medium (m^2/s)
mobility = 20n	Mobility of the species in the medium (m^2/Vs)

2.3.8 Electrokinetic Two Species Elbow

This template models electrokinetic transport of two species along an elbow channel. The channel contains a medium in which each species has a diffusivity and a mobility. There is an electric field along the length of the channel, expressed in volts/meter. Each species enters the channel as a band whose concentration versus distance is approximated as a gaussian distribution.

When connecting the electrostatic bend elements, use the right-handed (RH) or left-handed (LH) elements in the proper orientation. Do not flip these elements - only rotate them. Note that a right-handed element is different from a flipped left-handed element. If a bend element is flipped, it will not connect to the correct pins, and will result in errors in the output. Saber will not object to "height_out" being connected to "time_in".

The effect of the elbow is captured by a single parameter, alpha, where the full-width-half-maximum (fwhm) of a band after the bend is

fwhm_exit = alpha + fwhm_s

where alpha is an additional width caused by distortion due to the bend, and fwhm_s is the full-width-half-maximum of the band after traversing a straight channel of equivalent length. The length of the path is the sum of two leg_lengths and one 90 degree bend of radius bend_radius. The alpha for each species could be different, but in most applications both alpha1 and alpha2 are going to be set to the same value.

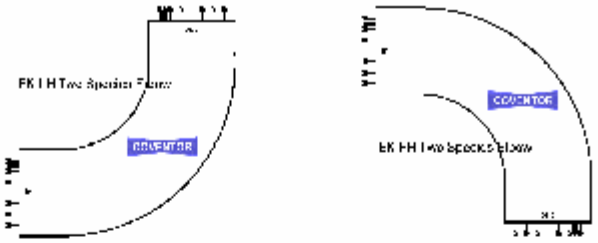
The input pins denote the three quantities necessary to define each gaussian: height, width and time. The height is the amplitude of the gaussian, the width is the full-width at half-maximum (fwhm) of the gaussian, and the time is the time when the gaussian enters the channel. The output pins denote the same quantities at the exit. Mobilities, diffusivities and electric field are assumed to be constant along the channel. DC operating point analysis of this model will generate the final state of the system: time the band enters and exits the channel, widths (fwhm, sigma, 1/e width) as the band enters and exits the channel, height as band enters and exits the channel, and velocity of the band. Tip: check the value of time_out of the last element in the channel to determine how long to run a transient analysis.

The two species have different mobilities and diffusivities. The separation of the two species at the exit is determined, and shown in the output signals, and can be used for a cross-over plot.

Transient analysis will produce quantities versus time since each band resides in the channel. Signals are height, widths, and position. The concentration profile of the band in time is also output as band_input and band_output. To view band_input and band_output clearly, the timestep must be reduced to a value approximately 1e-6 to1e-8 times the residence time. Use a large timestep during testing of the simulation until all desired settings are achieved. Then reduce the timestep until the gaussian bands become visible. The first run in transient analysis should have "End Time" set to the value of time_out of the last element in the channel.

Using the calculator, the band_input and band_output could each be plotted versus position to show the concentration profile versus distance, rather than time. For example, select and place the two signals band_output and position into the calculator. Select Wave->f(x) and select "Graph X".

Symbol Name: ek_LH_two_elbow
Ek_LH_two_elbow



Input Ports	Description
height_in1	height in
fwhm_in1	full-width-half_maximum in (meters)
time_in1	time when band enters (s)
height_in2	height in
fwhm_in2	full-width-half_maximum in (meters)
time_in2	time when band enters (s)

Output Ports	Description
height_out1	height out
fwhm_out1	full-width-half-maximum out (meters)
time_out1	time when band reaches exit
height_out2	height out
fwhm_out2	full-width-half-maximum out (meters)
time_out2	time when band reaches exit

User Input	Description
alpha1 = 0	Lumped effect of bend on species 1 (alpha=0 is ideal)
alpha2 = 0	Lumped effect of bend on species 2
leg_length = 0	Length of leg at each end of bend (m)
bend_radius = 1m	Radius of elbow (m)
electric_field = 10k	Electric field driving EK flow (V/m)
diffusivity1 = 5p	Diffusivity of the first species in the medium (m^2/s)
mobility1 = 20n	Mobility of the first species in the medium (m^2/Vs)
diffusivity2 = 5p	Diffusivity of the second species in the medium (m^2/s)
mobility2 = 20n	Mobility of the second species in the medium (m^2/Vs)

2.3.9 Electrokinetic Two Species Straight Channel

This template models electrokinetic transport of two species along a straight channel. The channel contains a medium in which each species has a diffusivity and a mobility. There is an electric field along the length of the channel, expressed in volts/meter. Each species enters the channel as a band whose concentration versus distance is approximated as a gaussian distribution.

The input pins denote the three quantities necessary to define each gaussian: height, width, and time. The height is the amplitude of the gaussian, the width is the full-width at half-maximum (fwhm) of the gaussian, and the time is the time when the gaussian enters the channel. The output pins denote the same quantities at the exit. Mobility, diffusivity, and electric field are assumed to be constant along the channel.

DC operating point analysis of this model will generate the final state of the system: time the band enters and exits the channel, widths (fwhm, sigma, 1/e width) as the band enters and exits the channel, height as band enters and exits the channel, and velocity of the band. Tip: check the value of time_out of the last element in the channel to determine how long to run a transient analysis.

The two species have different mobilities and diffusivities. The separation of the two species at the exit is determined and shown in the output signals. It can be used for a cross-over plot. Transient analysis will produce quantities versus time, as the band resides in the channel. Signals are height, widths, and position. The concentration profile of the band in time is also output as band_input and band_output. To view band_input and band_output clearly, the timestep must be reduced to a value approximately 1e-6 to 1e-8 times the residence time. Use a large timestep during testing of the simulation until all desired settings are achieved. Then reduce the timestep until the gaussian bands become visible. The first run in transient analysis should have "End Time" set to the value of time_out of the last element in the channel.

Using the calculator, the band_input and band_output could each be plotted versus position to show the concentration profile versus distance, rather than time. For example, select and place the two signals band_output1 and position1 into the calculator. Select Wave->f(x) and select "Graph X".

Symbol Name: ek_two_straight

Input Ports	Description
height_in1	height in
fwhm_in1	full-width-half_maximum in (meters)
time_in1	time when band enters (s)
height_in2	height in
fwhm_in2	full-width-half_maximum in (meters)
time_in2	time when band enters (s)

Output Ports	Description
height_out1	height out
fwhm_out1	full-width-half-maximum out (meters)
time_out1	time when band reaches exit
height_out2	height out
fwhm_out2	full-width-half-maximum out (meters)
time_out2	time when band reaches exit

User Input	Description
channel_length = 50m	Length of separation channel (m)
electric_field = 10k	Electric field driving EK flow (V/m)
diffusivity1 = 5p	Diffusivity of the species in the medium (m^2/s)
mobility1 = 20n	Mobility of the species in the medium (m^2/Vs)
diffusivity2 = 5p	Diffusivity of the species in the medium (m^2/s)
mobility2 = 20n	Mobility of the species in the medium (m^2/Vs)

2.3.10 Electrokinetic Two Species U-Bend

This template models electrokinetic transport of two species along a u-bend channel. The channel contains a medium in which each species has a diffusivity and a mobility. There is an electric field along the length of the channel, expressed in volts/meter. Each species enters the channel as a band whose concentration versus distance is approximated as a gaussian distribution. When connecting the electrostatic bend elements, use the right-handed (RH) or left-handed (LH) elements in the proper orientation. Do not flip these elements - only rotate them. Note that a right-handed element is different from a flipped left-handed element. If a bend element is flipped, it will not connect to the correct pins, and will result in errors in the output. Saber will not object to "height_out" being connected to "time_in".

The effect of the u-bend is captured by a single parameter, alpha, where the full-width-half-maximum (fwhm) of a band after the bend is

fwhm_exit = alpha + fwhm_s

where alpha is an additional width caused by distortion due to the bend, and fwhm_s is the full-width-half-maximum of the band after traversing a straight channel of equivalent length. The length of the path is the sum of two leg_lengths and one 180 degree bend of radius bend_radius. The alpha for each species could be different, but in most applications both alpha1 and alpha2 are going to be set to the same value.

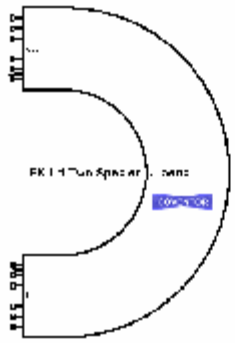
The input pins denote the three quantities necessary to define each gaussian: height, width and time. The height is the amplitude of the gaussian, the width is the full-width at half-maximum (fwhm) of the gaussian, and the time is the time when the gaussian enters the channel. The output pins denote the same quantities at the exit. Mobilities, diffusivities, and electric field are assumed to be constant along the channel.

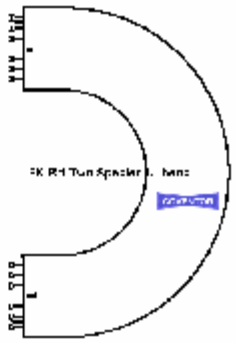
DC operating point analysis of this model will generate the final state of the system: time the band enters and exits the channel, widths (fwhm, sigma, 1/e width) as the band enters and exits the channel, height as band enters and exits the channel, and velocity of the band. Tip: check the value of time_out of the last element in the channel to determine how long to run a transient analysis. The two species have different mobilities and diffusivities. The separation of the two species at the exit is determined, and shown in the output signals, and can be used for a cross-over plot. Transient analysis will produce quantities versus time, as each band resides in the channel. Signals are height, widths, and position. The concentration profile of the band in time is also output as band_input and band_output. To view band_input and band_output clearly, the timestep must be reduced to a value approximately 1e-6 to 1e-8 times the residence time. Use a large timestep during testing of the simulation until all desired settings are achieved. Then reduce the timestep until the gaussian bands become visible. The first run in transient analysis should have "End Time" set to the value of time_out of the last element in the channel. Using the calculator, the band_input and band_output could each be plotted versus position, to show the concentration profile versus distance,

rather than time. For example, select and place the two signals band_output and position into the calculator. Select Wave->f(x) and select "Graph X".

Symbol Name: ek_lh_two_u_bend

ek_rh_two_u_bend





Input Ports	Description
height_in1	height in
fwhm_in1	full-width-half_maximum in (meters)
time_in1	time when band enters (s)
height_in2	height in
fwhm_in2	full-width-half_maximum in (meters)
time_in2	time when band enters (s)

Output Ports	Description
height_out1	height out
fwhm_out1	full-width-half-maximum out (meters)
time_out1	time when band reaches exit
height_out2	height out
fwhm_out2	full-width-half-maximum out (meters)
time_out2	time when band reaches exit

User Input	Description
alpha1 = 0	Lumped effect of bend on species 1 (alpha=0 is ideal)
alpha2 = 0	Lumped effect of bend on species 2
leg_length = 0	Length of leg at each end of bend channel (m)
bend_radius = 1m	Radius of u-bend (m)
electric_field = 10k	Electric field driving EK flow (V/m)
diffusivity1 = 5p	Diffusivity of the first species in the medium (m^2/s)
mobility1 = 20n	Mobility of the first species in the medium (m^2/Vs)
diffusivity2 = 5p	Diffusivity of the second species in the medium (m^2/s)
mobility2 = 20n	Mobility of the second species in the medium (m^2/Vs)

2.3.11 Electrokinetic U-Bend

This template models electrokinetic transport of a species along a u-bend channel. The channel contains a medium in which the species has a diffusivity and a mobility. There is an electric field along the length of the channel, expressed in volts/meter. The species enters the channel as a band whose concentration versus distance is approximated as a gaussian distribution. When connecting the electrostatic bend elements, use the right-handed (RH) or left-handed (LH) elements in the proper orientation. Do not flip these elements - only rotate them. Note that a right-handed element is different from a flipped left-handed element. If a bend element is flipped, it will not connect to the correct pins, and will result in errors in the output. Saber will not object to "height_out" being connected to "time_in".

The effect of the u-bend is captured by a single parameter, alpha, where the full-width-half-maximum (fwhm) of a band after the bend is

fwhm_exit = alpha + fwhm_s

where alpha is an additional width caused by distortion due to the bend, and fwhm_s is the full-width-half-maximum of the band after traversing a straight channel of equivalent length. The length of the path is the sum of two leg_lengths and one 180 degree bend of radius bend_radius.

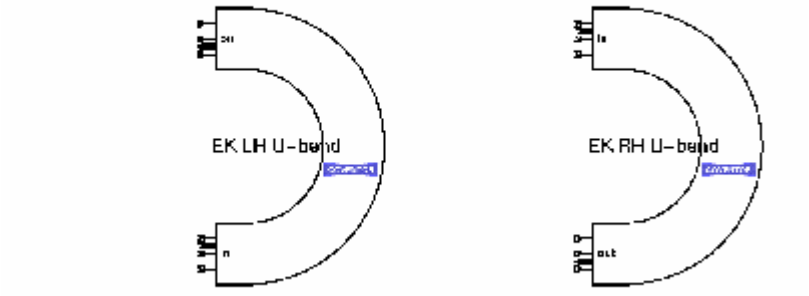
The input pins denote the three quantities necessary to define the gaussian: height, width, and time. The height is the amplitude of the gaussian, the width is the full-width at half-maximum (fwhm) of the gaussian, and the time is the time when the gaussian enters the channel. The output pins denote the same quantities at the exit. Mobility, diffusivity, and electric field are assumed to be constant along the channel.

DC operating point analysis of this model will generate the final state of the system: time the band enters and exits the channel, widths (fwhm, sigma, 1/e width) as the band enters and exits the channel, height as band enters and exits the channel, and velocity of the band. Tip: check the value of time_out of the last element in the channel to determine how long to run a transient analysis.

Transient analysis will produce quantities versus time since the band resides in the channel. Signals are height, widths, and position. The concentration profile of the band in time is also output as band_input and band_output. To view band_input and band_output clearly, the timestep must be reduced to a value approximately 1e-6 to 1e-8 times the residence time. Use a large timestep during testing of the simulation until all desired settings are achieved. Then reduce the timestep until the gaussian bands become visible. The first run in transient analysis should have "End Time" set to the value of time_out of the last element in the channel. Using the calculator, the band_input and band_output could each be plotted versus position to show the concentration profile versus distance, rather than time. For example, select and place the two signals band_output and position into the calculator. Select Wave->f(x) and select "Graph X".

Symbol Name: ek_rh_u_bend

ek_lh_u_bend



Input Ports	Description
height_in	height in
fwhm_in	full-width-half_maximum in (meters)
time_in	time when band enters (s)

Output Ports	Description
height_out	height out
fwhm_out	full-width-half-maximum out (meters)
time_out	time when band reaches exit

User Input	Description
alpha = 0	Effective distance of a bend due to the bend (alpha=0 is ideal)
leg_length = 0	Length of leg at each end of bend (m)
bend_radius = 1m	Radius of u-bend (m)
electric_field = 10k	Electric field driving EK flow (V/m)
diffusivity = 5p	Diffusivity of the species in the medium (m^2/s)
mobility = 20n	Mobility of the species in the medium (m^2/Vs)

2.3.12 Elbow Channel

This template models fluid flow through a rigid elbow channel of three cross-sectional shapes: circular, rectangular, and d_shaped. D-shape cross sections are defined as follows:

length of long straight side of "D" = width+2*d

length of short straight side of "D" = width

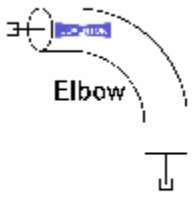
each curved part of "D" is quarter circle of radius d

There is a straight section of channel at each end of the elbow of length 0.25*radius in order for the flow to be fully developed. Factor in the channel length when calculating the total channel path. The total path in the elbow is therefore

length = radius*(pi/2 + 1/2).

The true flow may not be laminar if the Reynolds number exceeds 2000. Laminar flow is assumed in this template.

Symbol Name: elbow



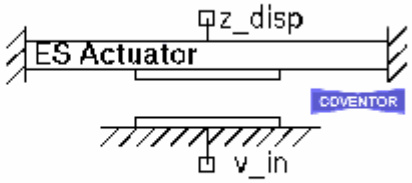
Ports: p1 (Hydraulic)
p2 (Hydraulic)

User Input	Description
d	Inner diameter or depth
width=undef	width of D-channel or rectangle
radius	radius (m)
viscosity	local viscosity
density	local density
cross section	circular, rectangular, d_shaped

2.3.13 Electrostatic Actuator

An electrostatic actuator models the displacement of a membrane that deforms due to an electrostatic force induced by a capacitor. The membrane is composed of two connected beams, and its vertical displacement is that of the beams interconnection node. Because only vertical displacement is needed, the other translation and rotation degrees of freedom of the beams are grounded. The capacitance to translation converter (transcaptran) has voltage as input and displacement as output. Refer to parallel plate capacitor for more information.

Symbol Name: ES_actuator



Ports: Z-disp (mechanical)
V_in (electric)

2.3.14 FlowMM Resistor and Inertor

This template is used in conjunction with FlowMM, which produces the data files *res_tlu_data.ai_dat* and *inert_array_data.ai_dat*. FlowMM calculates pressure versus flow rate with one parameter. The file *res_tlu_data.ai_dat* is a table with three columns, where the columns are labeled in order as: pressure drop, parameter, flow rate and the data is in MKS units (meters, kilograms, seconds). The field "datafile" can be changed to a user-specified file name, where the default is res_tlu_data.ai_dat.

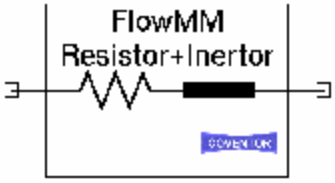
The file inert_tlu_data.ai_dat is a table with three columns, where the columns are labeled in order: pressure drop, parameter, and time_constant. The data is in MKS units (meters, kilograms, seconds). The field "datafile" can be changed to a user-specified file name, where the default is *inert_tlu_data.ai_dat*.

This model uses the data files to represent a generic flow channel with resistance and inertance, where the resistance is a function of the flow rate. This is the general case of the diodic_valve template.

The resistance can be multiplied by a factor, multiplier_res, using the same data file for a device whose properties have changed when the resistance is known to be linearly proportional to that property. Note that P=RQ, where P is pressure drop, R is resistance, and Q is flow rate. Multiplying the resistance by 0.5 doubles the flow rate.

The inertance can be multiplied by a factor, multiplier_inert, using the same data file for a device whose properties have changed when the inertance is known to be linearly proportional to that property. Note that P=IdQ/dt, where P is pressure drop, I is inertance, and Q is flow rate.

Symbol Name: flowmm_resinert



Ports: p1 Hydraulic
p2 Hydraulic

User Input: parameter=0
res_datafile="res_tlu_data.ai_dat"
inert_datafile="inert_tlu_data.ai_dat"
multiplier_res=1
multiplier_inert=1

2.3.15 FlowMM Resistor

This template is used in conjunction with FlowMM, which produces the data file *res_tlu_data.ai_dat*. FlowMM calculates pressure versus flow rate with one parameter. The file *res_tlu_data.ai_dat* is a table with three columns, where the columns are labeled in order: pressure drop, parameter, and flow rate. The data is in MKS units (meters, kilograms, seconds). The field "datafile" can be changed to a user-specified file name, where the default is *res_tlu_data.ai_dat.*

This model uses the data files to represent a generic flow channel with resistance, where the resistance is a function of the flow rate. This is the general case of the diodic_valve template. The resistance can be multiplied by a factor, multiplier_res, using the same data file for a device whose properties have changed when the resistance is known to be linearly proportional to that property. Note that P=RQ, where P is pressure drop, R is resistance, and Q is flow rate. To double the flow rate, multiply the resistance by 0.5.

Symbol Name: flowmm_resistor

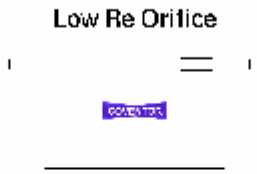
Ports: p1 (Hydraulic)
p2 (Hydraulic)

User Input	Description
parameter	100 um, pipe diameter
Table_lookup	Data file specification, multiplier_res and multiplier_inert

2.3.16 Low Re Orifice

This template models fluid flow through a sharp-edged orifice at Reynolds numbers less than 10. Flow passes from a pipe of inner diameter d_in through a circular orifice of diameter d_orifice in a flat plate of negligible thickness. When connecting pipes to the orifice symbol, do not account for any thickness of the orifice plate nor any length of the d_in entry. The ratio of d_in to d_orifice must be greater than 10.

Symbol Name: low_re_orif



Ports: p1 (Hydraulic)
p2 (Hydraulic)

User Input	Description
d_in	Inlet pipe diameter
d_orifice	Orifice diameter
viscosity	Viscosity
density	Density

2.3.17 Meander

This template models fluid flow from port p1 to p2 through a meandering channel. The shape is composed of 90 degree elbows and 180 degree u-bends, whose radii (measured from the centerline of the channel) are defined by the user. The rest of the path is made up of straight sections that connect the two ports. All channels are rigid.

This meander is designed to fit in a footprint of length footpr_l and width footpr_w, where the footprint is the smallest rectangle enclosing the whole path. The ports are centered on the width even if there is one u-bend. Zero u- bends is equivalent to a straight channel of length footpr_l. The user defines the number of u-bends. The rest of the channel is assumed to fit symmetrically between the two ports. Error messages will result if the number of u-bends and the bend radii requested are incompatible with the footprint.

As with the other templates, there are three cross-sectional shapes: circular, rectangular and d_shaped. D-shape cross sections are defined as follows:

length of long straight side of "D" = xsect_w+2*xsect_d

length of short straight side of "D" = xsect_w

each curved part of "D" is quarter circle of radius xsect_d

The true flow may not be laminar if the Reynolds number exceeds 2000. Laminar flow is assumed in this template.

Symbol Name: meander

Ports p1 (Hydraulic)

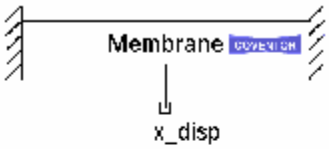
p2 (Hydraulic)

User Input	Description
xsect_d	Inner diameter or depth of cross-section
xsect_w	width of D-channel or rectangle cross-section
footpr_l	length of footprint (between ports)
footpr_w	width of footprint
num_ubend	number of u_bends
ubend_radius	radius of u_bends
elbow_radius	radius of elbows
viscosity	local viscosity
density	local density
cross section	circular, rectangular, d_shaped

2.3.18 Edge Fixed Membrane

This template is a one-dimensional model of a thin plate subject to fixed boundary conditions on all edges. The displacement of the center of the membrane is normal to the plate and is represented by the translational_pos pin, x_disp. The mass and spring constants of the membrane are tuned to match a circular or rectangular plate.

Symbol Name: membrane



Port: x_disp (mechanical)

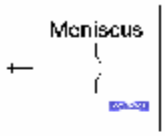
User Input	Description
d	diameter of circle or depth of rectangle
width=undef	width of rectangle
thickness	membrane thickness
youngs_modulus	modulus of elasticity
poisson_ratio	poisson ratio for membrane material (dimensionless)
density	local density
cross section	circular, rectangular

2.3.19 Spherical Droplet

This template models the growth of spherical droplets of fluid issuing from a circular sharp-edged nozzle of diameter d_nozzle. The drop is assumed to be a spherical section at all times, where the radius of curvature varies according to the system. The drop is considered to cut off when the diameter of the spherical section outside the nozzle is equal to drop_threshold times the nozzle diameter. After cutting off, the meniscus becomes a spherical cap of volume cut_ratio times that of a hemisphere.

Pinch_duration allows the user to specify some time between the cut-off and the cut_ratio shape. However, the volume continues to change during this time, so after pinch_duration has elapsed, the pressure may jump to correspond to the volume.

Symbol Name: meniscus



Port: p (hydraulic)

User Input	Description
Surface_tension = 0.0734	surface tension
D_nozzle	inner diameter of nozzle
Drop_threshold = 1.4	ratio of drop radius to nozzle radius when drop is cut off
cut_ratio = 0.5	ratio of volume remaining meniscus after cutoff to volume of a hemisphere
pinch_duration	time between cut_off and cut_ratio shape

2.3.20 Spherical Droplet – Two Port

This template models the growth of spherical droplets of fluid issuing from a circular sharp-edged nozzle of diameter d_nozzle. The drop is assumed to be a spherical section at all times, where the radius of curvature varies according to the system. The drop is considered to cut off when the diameter of the spherical section outside the nozzle is equal to drop_threshold times the nozzle diameter. After cutting off, the meniscus becomes a spherical cap of volume cut_ratio times that of a hemisphere.

Pinch_duration allows the user to specify some time between the cut-off and the cut_ratio shape. However, the volume continues to change during this time, so after pinch_duration has elapsed, the pressure may jump to correspond to the volume. The second port allows droplet to evolve due to a vacuum.

Symbol Name: meniscus_atm

Port: p1 (hydraulic)
p2 (hydraulic)

User Input	Description
surface_tension=73.4m	surface tension
d_nozzle	inner diameter of nozzle
drop_threshold = 1.4	ratio of drop diameter to nozzle diameter when drop cuts off
cut_ratio = 0.5	ratio of volume of remaining meniscus after cut-off to volume of a hemisphere
pinch_duration = 0	time between cut-off and cut_ratio shape

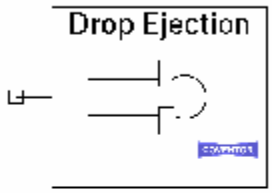
2.3.21 Head and Neck Model of Droplet

This template models the growth of spherical droplets of fluid issuing from a circular sharp-edged nozzle. The drop is assumed to be a spherical section at first, where the radius of curvature varies according to the system.

When the drop volume reaches a critical value, the head of the drop is assumed to pull away from the nozzle. A neck begins to form between the nozzle and the drop head, and grows in length at a fixed velocity equal to the average velocity of the head. The volume of the neck is determined by the flow_rate into the element, so the radius of the neck can be determined. During the neck stage, the pressure the meniscus element exerts on the system is surface_tension/radius, or that of a cylindrical neck. The neck pinches off when the radius drops below a critical threshold.

After pinching off, the meniscus that remains is flat and at zero velocity. Ejected_volume tracks the total volume ejected including past drops. The total volume includes the head volume plus the entire neck volume.

Symbol Name: meniscus_neck



Port: p (hydraulic)

User Input	Description
surface_tension=73.4m	surface tension
d_nozzle	inner diameter of nozzle
head_threshold = 1.4	ratio of drop diameter to nozzle diameter when head is formed
pinch_threshold = 0.1	ratio of neck diameter to nozzle diameter when neck pinches off
cut_ratio = 0.5	ratio of volume of remaining meniscus after cut-off to volume of a hemisphere

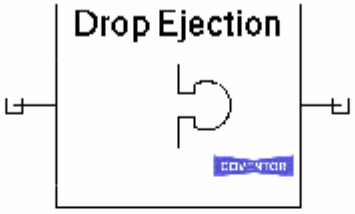
2.3.22 Head and Neck Model of Droplet – Two Port

This template models the growth of spherical droplets of fluid issuing from a circular sharp-edged nozzle. The drop is assumed to be a spherical section at first, where the radius of curvature varies according to the system.

When the drop volume reaches a critical amount, the head of the drop is assumed to pull away from the nozzle. A neck begins to form between the nozzle and the drop head, and grows in length at a fixed velocity equal to the average velocity of the head. The volume of the neck is determined by the flow_rate into the element, so the radius of the neck can be found. During the neck stage, the pressure the meniscus element exerts on the system is surface_tension/radius, or that of a cylindrical neck. The neck pinches off when the radius drops below a critical threshold.

After pinching off, the meniscus that remains is flat at zero velocity. The parameter, ejected_volume tracks the total volume ejected including past drops. The total volume includes the head volume plus the entire neck volume. Second port allows drop to evolve due to vacuum.

Symbol Name: meniscus_neck_atm



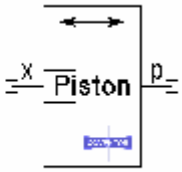
Ports: p1 (hydraulic)
p2 (hydraulic)

User Input	Description
surface_tension=73.4m	surface tension
d_nozzle	inner diameter of nozzle
head_threshold = 1.4	ratio of drop diameter to nozzle diameter when head is formed
pinch_threshold = 0.1	ratio of neck diameter to nozzle diameter when neck pinches off
cut_ratio = 0.5	ratio of volume of remaining meniscus after cut-off to a hemisphere

2.3.23 Piston

This template models the pressure imparted on a fluid by a piston acted upon by a force. The piston undergoes a translation, $x-x_0$, and the flow pressure difference is $p-p_0$, where x_0 and p_0 are ground. If the fluid domain requires a rescaling into microns, the property length_units can be set to microns to match.

Symbol Name: Piston



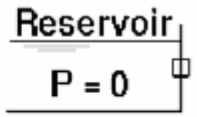
Ports: p hydraulic

x mechanical

User Input	Description
area	area of piston
length_units	select units for fluid side of piston symbol (meters or microns)

2.3.24 Reservoir

Reservoir serves the same purpose as a ground.

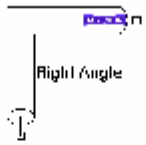


Symbol Name: Reservoir

2.3.25 Right Angle Channel

This template models fluid flow through a rigid channel with a sharp right angle and a rectangular cross-section. The length of each leg is four times its width. The width is the dimension in the plane of the right angle. The Reynolds number should not exceed about 100, which is the upper limit of the model.

Symbol Name: right_angle



Ports: p1 Hydraulic

p2 Hydraulic

User Input	Description
width	channel width in plane of right angle
Height	channel height
viscosity	viscosity
density	density
cross_section	rectangular(width, height)

2.3.26 Straight Channel

This template models fluid flow through a rigid channel of three cross-sectional shapes: circular, rectangular and d_shaped. D-shape cross sections are defined as follows:

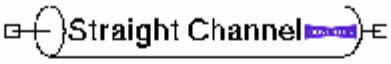
length of long straight side of "D" = width+2*d

length of short straight side of "D" = width

each curved part of "D" is quarter circle of radius d

The true flow may not be laminar if the Reynolds number exceeds 2000. Laminar flow is assumed in this template.

Symbol Name: straight_channel



Ports: p1 Hydraulic

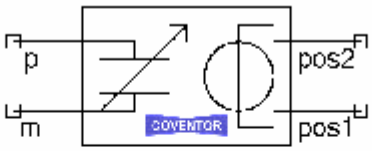
p2 Hydraulic

User Input	Description
d	Inner diameter or depth
width=undef	width of D-channel or rectangle
length	length (m)
viscosity	local viscosity
density	local density
cross section	circular, rectangular, d_shaped

2.3.27 Parallel-Plate Capacitor

This template represents a transducer between capacitance and translation. It models the electrostatic attraction force between two plates separated by a dielectric in a gap, where a given voltage difference is applied to the plates.

Symbol Name: Transcaptran



Ports	Description
p	electrical
M	electrical
pos1	mechanical
pos2	mechanical

User Input	Description
area	Area of electrodes of capacitor
Epr	Relative permitivity in capacitor gap
Gap	Nominal gap between electrodes
K	Capacitance correction factor (fringing fields)

2.3.28 U-Bend Channel

This template models fluid flow through a rigid u_bend channel of three cross-sectional shapes: circular, rectangular and d_shaped. D-shape cross sections are defined as follows:

length of long straight side of "D" = width+2*d

length of short straight side of "D" = width

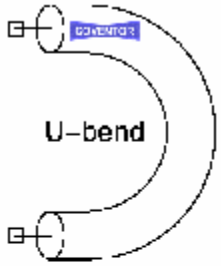
each curved part of "D" is quarter circle of radius d

There is a straight section of channel at each end of the u_bend of length 0.25*radius in order for the flow to be fully developed. Be sure to factor in that length of channel when considering the total channel path. The total path in the u_bend is therefore

length = radius*(pi + 1/2).

The true flow may not be laminar if the Reynolds number exceeds 2000. Laminar flow is assumed in this template.

Symbol Name: u_bend



Ports: p1 Hydraulic
p2 Hydraulic

User Input	Description
d	Inner diameter or depth
width=undef	width of D-channel or rectangle
radius	radius of the U-Bend
viscosity	local viscosity
density	local density
cross section	circular, rectangular, d_shaped

Section 3: Fluidics System Modeling Tutorial

3.1: Overview

This tutorial is an overview of the design optimization of a microfluidic network for the investigation of enzyme inhibition. The fluidic design (i.e. channel sizes) will be optimized based on the required flow rates and mixing ratios of the different species. The influence of etch depth is investigated on a system model level, allowing fast design iterations.

3.1.1 Background

New drugs can be developed using the High Throughput Screening (HTS) methodology. In this approach, large libraries of typically tens of thousands of drug candidates are synthesized and then tested against the target of interest (i.e. cell membrane receptor molecule, enzymes etc.). In this screening phase, a number of drug candidates (or 'leads') emerge, which show a strong interaction with the target. These candidates are subject to further evaluation.

In both the synthesizing phase and the screening phase, miniaturization and parallel implementation of processes are highly beneficial since these factors tend to decrease development times. The subject for this tutorial is a single, pressure-driven microfluidic network (see figure 3-1).

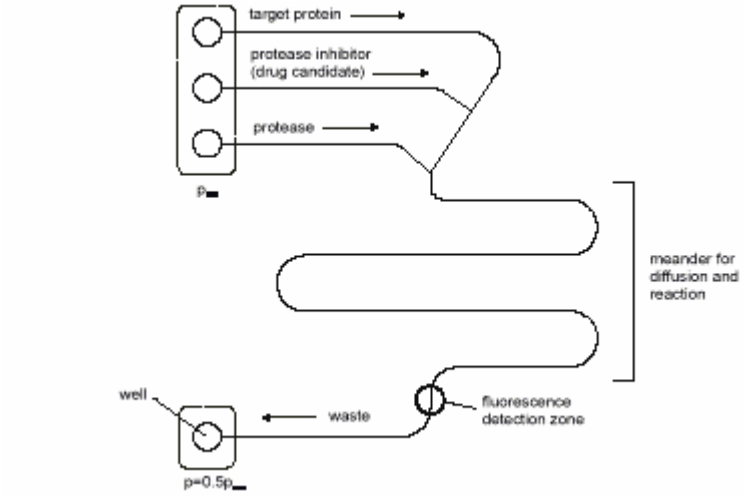


Figure 3-1 Layout of a Microfluidic Network for Enzyme Inhibition Study

In this network, the target protein is mixed with protease (i.e. enzyme that cleaves the target protein) and the protease inhibitor (the drug candidate). The three liquids are driven at constant speed through the network by the application of suction at the waste well (0.5 atmosphere). Mixing and reaction take place in the meander and the reaction mixture is optically investigated at the end.

It is assumed that the inlet wells are at atmospheric pressure and that the wells do not have any resistance. The design is implemented by isotropic etching of glass (D-shaped channel cross-section) with the same etch depth of 20μm in all channels. Finally it is assumed that all liquids are aqueous solutions at room temperature and that the chemical reactions are rate limited (i.e. diffusion proceeds relatively quickly).
In a later phase of the design, a number of these individual units can be put together in an array format to allow the parallel screening of a large number of drug candidates (see figure 3-2).

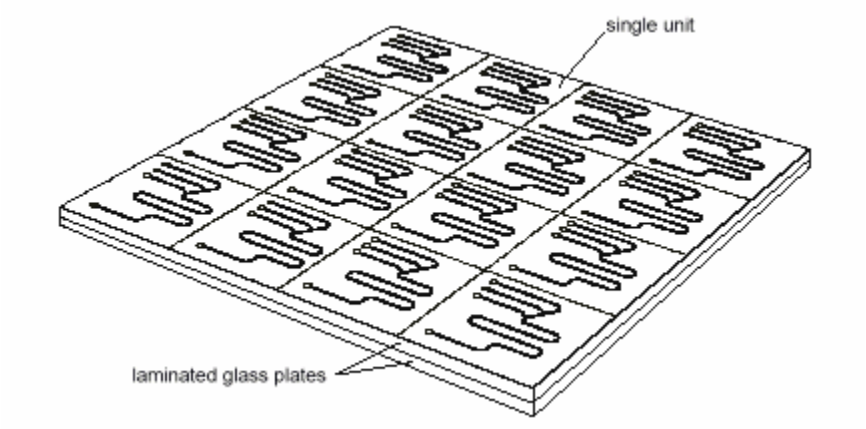


Figure 3-2 Array Format for Parallel Screening

3.1.2 Design Requirements

The following requirements should be met by the design:

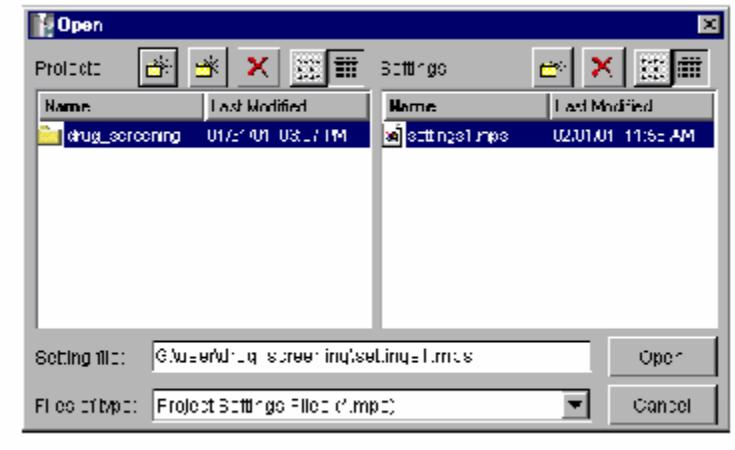
- Pyrex® substrate, isotropic wet etching (D-shaped cross-sections),
- Initial etch depth 20μm,
- At system outlet 0.5 bar (=50 kP) under pressure,
- Unit size 9x9 mm, total element size 8x8 mm,
- Radius of curvature of the centerline of the channels should be at least the width of the channel,
- Well volume 1 μl,
- Flow rate low enough to let system function for at least 60 s (total flow rate maximal 1μl/60 s=33.33 pl/s),
- Equal flow rate from protease and protease inhibitor wells (i.e. 8.33 pl/s) and twice the flow rate from the target protein well (16.66 pl/s),
- Minimum mask width 10 μm,
- Residence time in the meander is minimal 10 s to allow complete reaction,
- Assume liquid properties for water at 20 C.

3.2: First Design Pass - Building the Schematic (Part A)

The procedure for the first design pass is as follows.

1. Start CoventorWare. Be sure that Saber was installed (not installed by default).

2. Create a new project called “drug_screening”, and specify a settings file name “setting1.mps”. Note that under the project directory a schematics directory will be created that will contain your saved schematic file (.ai_sch).



3. Click on the **System Modeling** tab and then click the **Start MemSys** button to activate the Saber interface. The MemSys Sketch window will open (see Figure 3-3).

4. Click the red **Show/Hide SaberGuide** icon (icon 19 from the left), to show the SaberGuide buttons.

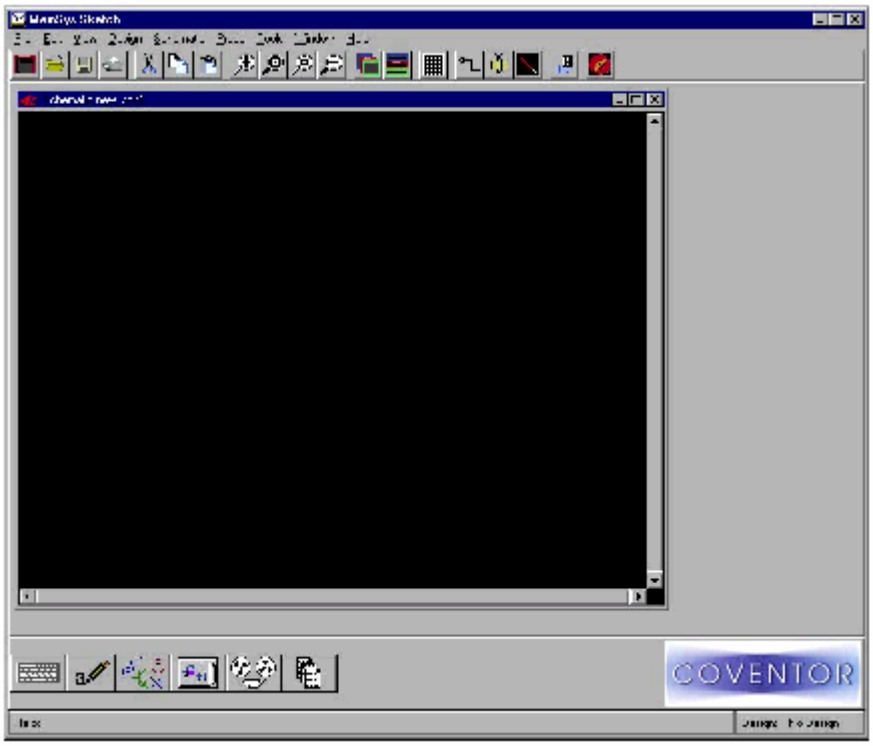


Figure 3-3 MemSys Sketch Window

5. Open the Parts Gallery window (see Figure 3-4).

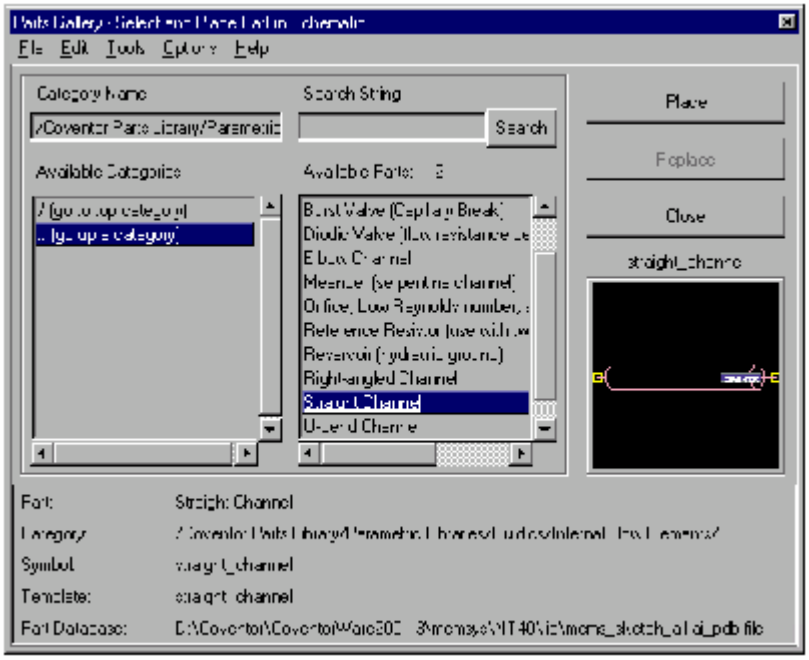


Figure 3-4 Parts Gallery Window

6. In the Parts Gallery window navigate to Coventor Parts Library/Parametric Libraries/Fluidics/Internal Flow Elements.

7. Select Straight Channel (i.e. the target protein channel) and click Place. You may need to move the Parts Gallery window away from MemSys Sketch window to see the part. Rotate the channel vertically using Schematic > Rotate > 270. Note that the flow direction is defined as positive from port P1 to port P2.

8. Place another Straight Channel (i.e. the protease inhibitor channel). Drag (using the left mouse button) the channel perpendicularly below and to the left of the first channel. Make sure that the two channels are connected (the small connecting box disappears).

9. Place and rotate a third Straight Channel vertically below the first channel.

10. Place a fourth Straight Channel (i.e. the protease channel) perpendicularly below and to the left of the third channel.

11. Select Zoom to Fit (icon 10 in the second row of buttons).

12. Continue to place the remaining fluid elements as shown in the diagram in Figure 3-5:

    - 1 Meander
    - 1 additional straight channel (5 total)
    - 3 Reservoirs (i.e. hydraulic ground)
    - 1 Pressure Source, Constant Ideal (located in Analogy Parts Library\Hydraulic\Hydraulic Sources; alternatively use the search option with template name pres_dc).
    - 1 Coventor symbol (Saber Include File) to set parameters (located in Coventor Parts Library/shared parts).
    - 1 Ground (located in the Analogy Parts Library).

Note: You can connect parts with a line by simply clicking on the port of each of the parts to be connected.

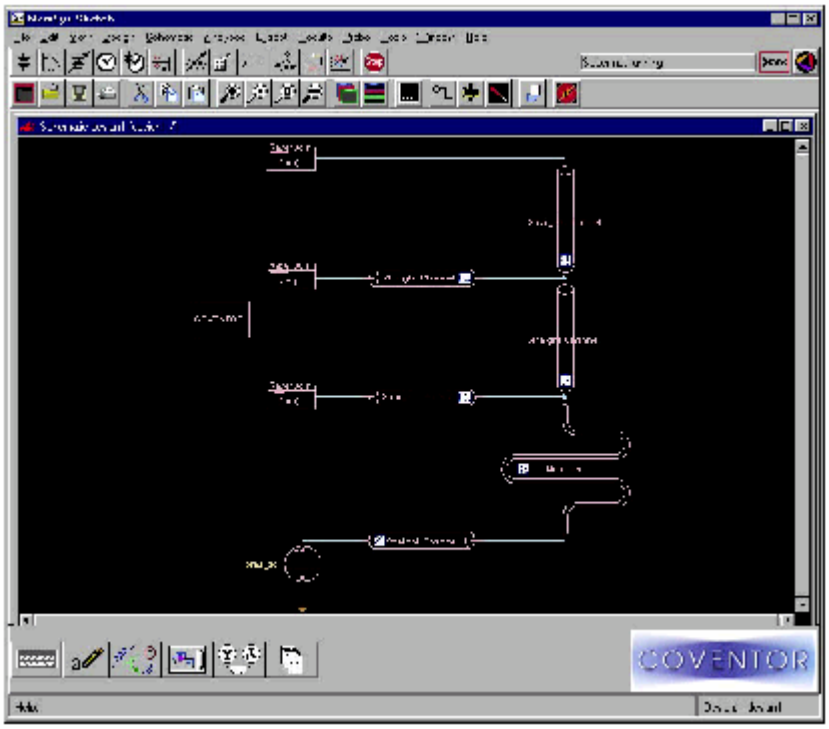


Figure 3-5 Fluid Elements

13. Close the Parts Gallery window and save your work as design1.ai_sch with **File > Save As > design1**. The default file name is new_sch1.

14. Set the dimensions for each element by double clicking on one of the elements and filling in the values in the table that opens. The values to be used are displayed in the enlarged MemSys Schematic shown in Figure 3-6.

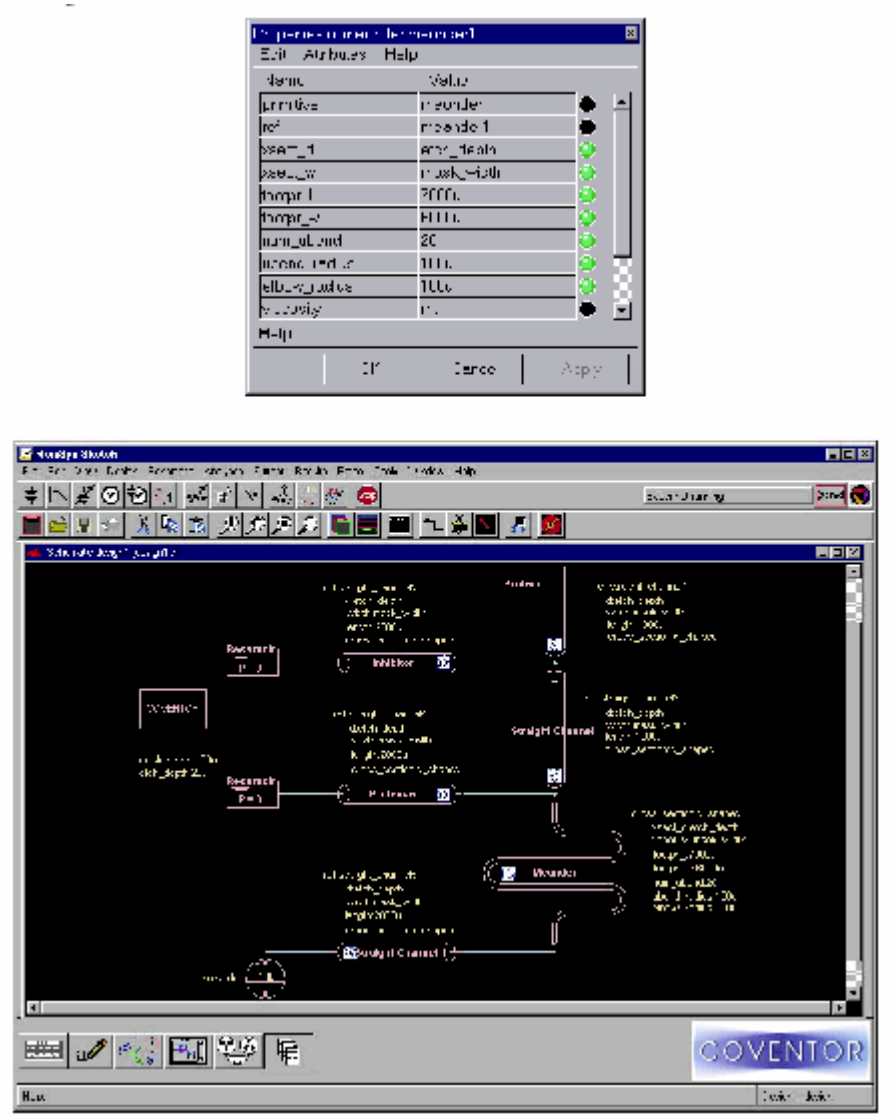


Figure 3-6 MemSys Schematic

15. Change the **ref labels** for the straight channels connected to the reservoirs as follows:

- Channel 1: Protein
- Channel 2: Inhibitor
- Channel 4: Protease
- Note that units are in SI. The symbol u is used to input the length in microns (e.g. 2000u). In this example a negative pressure of –50k (-0.5 atm) is set to draw fluid from each reservoir.
- The variable names etch_depth, mask_width, mu and rho will be defined in the Coventor symbol element.

16. Activate the display of both the name and value on the schematic by clicking on the black buttons to the right of the values. The button works in three modes; no display, name only, name and value.

17. Click **Apply, OK**. Repeat this for all of the remaining fluid elements.

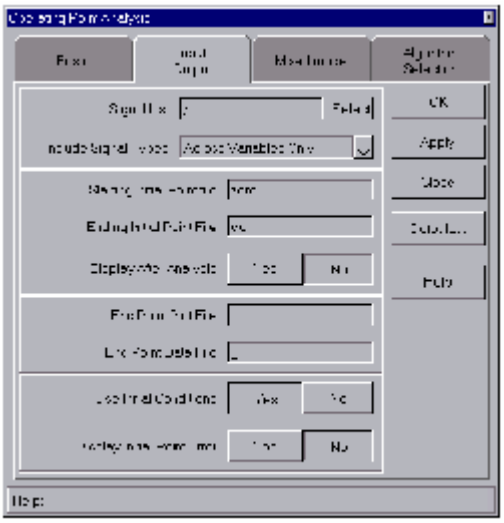
18. Double click on the Coventor symbol. Set the etch_depth to 20u by entering a new property and new value at the bottom of the table. Click **Apply, OK**. Set mask_width to 100u. Note that by not setting values for mu and rho the default properties values for water will be used.

19. Save your completed schematic; **File > Save.**

Initial Design Evaluation

20. Click on **Design > Netlist** (this creates a text input file with the extension .sin). View the transcript file for errors; **View > Show Netlister Transcript.** Click on **Design > Simulate** to start Saber.

21. The flow rates through the network can be calculated by running 'DC operating point analysis', which can be accessed by pulling down **Analyses > Operating Point > DC Operating Point** to open up the Operating Point Analysis window.



22. Click the **Input/Output** tab.

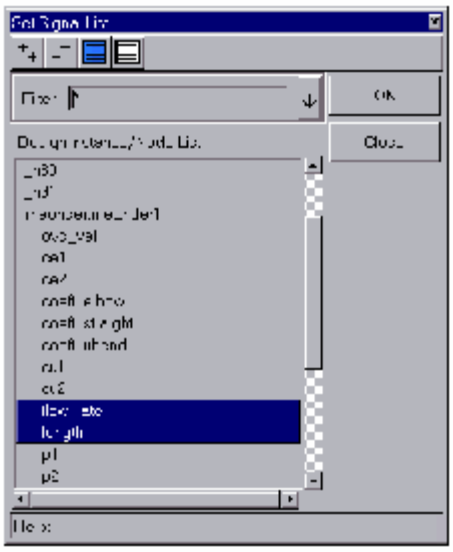
23. Click the **Select** button and then **Browse Design** to select the results of interest to display (alternatively choose **All Signals**, to display all results).

24. Double click on the fluid element name to display the variables for that element. Use the **Ctrl** key to select multiple results output:

25. Select **flow_rate, length, pressure_drop,** and **residence_time** for the meander.

26. Select **flow_rate** and **pressure_drop** for each of the three straight channels connected to the reservoirs.

27. Click **OK.**

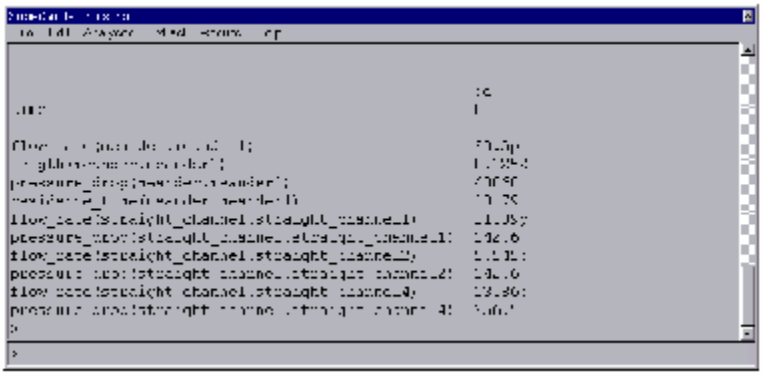


28. At the *Display After Analysis* option, click the **Yes** button.

29. Click **OK** to run the simulation.

30. Click the >cmd icon (top right of MemSys Sketch window) to bring up the SaberGuide Transcript window.

31. The results will be displayed in the transcript window. (Only the previously selected parameters are output).



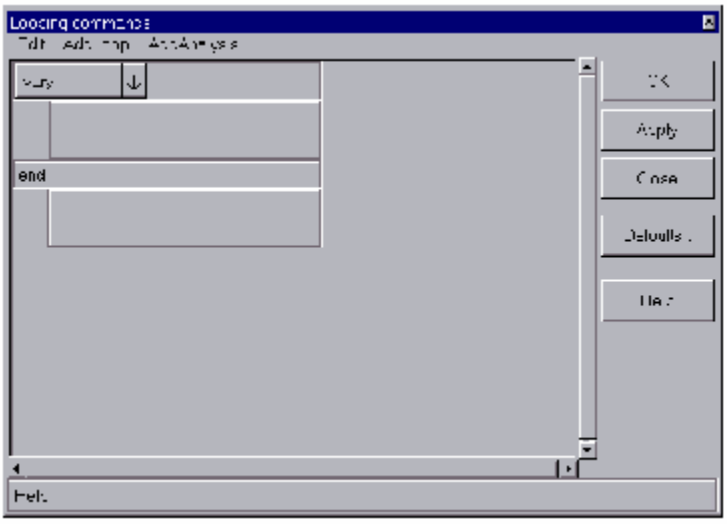
32. As can be seen, both the net flow rate (30.5 pl/s) and the residence time in the meander (10.79 s) match the design requirements. If further modification is required, the number of turns in the meander as well as the mask width may be changed.

It also follows that the ratio in flow rate between the target protein channel (channel 1) and protease inhibitor channel (channel 2) is 2:1, as desired (a direct result of the factor 2 ratio in length). To match the flow rate of the protease channel (channel 4), its width may be varied until it equals the flow rate of the protease inhibitor channel (channel 2). This will be demonstrated in the next section.

3.3: Matching the Mix Ratio (Part B)

The influence of the width of channel 4 can be determined by a 'Vary' analysis.

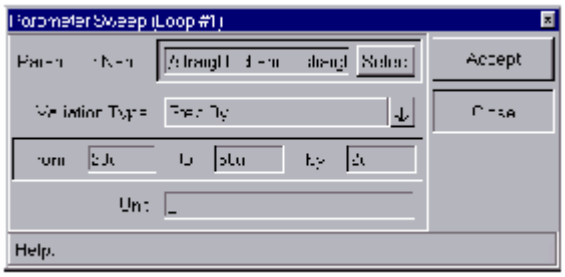
1. Pull down the Looping commands window: **Analyses > Parametric > Vary**.



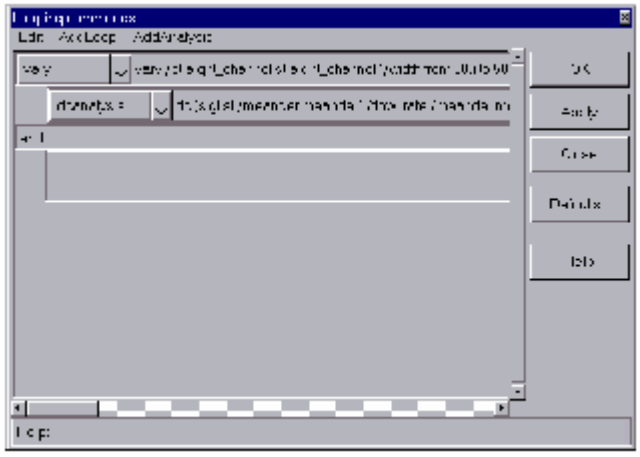
2. In the Looping commands window click the **vary** button and double click channel 4 (use **Select >Browse Design**). Select the parameter **width** and click **OK**.

3. Set the start value, end value and increment for the parameter sweep on channel width (from 20u to 50u by 2u).

4. Click **Accept.**



5. In the Looping commands Window pull down **AddAnalysis > Within Loops > DC Operating Point**.



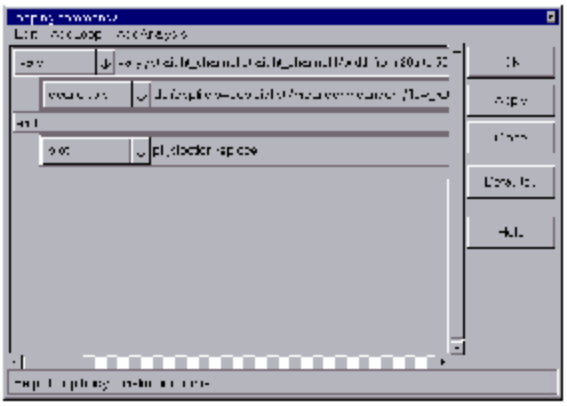
6. Click the **dcanalysis** button. Under the **Input/Output** tab set the End Point Plot File name to 'sweep'.

7. Verify the parameters of interest (flow rates in inlet channels), using **Select > Browse Design** as done in the previous section

8. Click **Accept.**

9. Pull down **AddAnalysis** > **After loop(s)** > **View Plotfiles in Scope**

10. Click **Plot** and select **Replace Plots** from the pull down list under **Plot Action**. Click **Accept.**



11. Click **OK** to run the simulation.

View the Results

12. After a few seconds the Memsys graphics window (Figure 3-7), and two windows containing the plot file (window labeled **Signal Manager**), and the flow_rate results (window labeled **design1.sweep**) will open.

13. Resize the graphics window and move the smaller windows to the side. Then select one of the flow_rate results from the list, and click **Plot**. To add another flow_rate result to the graph, select another result from the list, and click with the middle mouse inside the new graph area. If needed, the graphics window can be cleared with the *Clear* icon (icon 13 from the left).

14. Select the flow rate of channel 4 from the legend in the graphics window, and click the **At X Measurement** icon (icon 17 from the left)

15. If not done automatically, move the cursor to the point of intersection. At this point the flow rate in channel 4 equals the flow rate in channel 2. This occurs at a width of 29.955 µm, which is the required mask width of channel 4. Note that the flow rate of channel 1 is always twice the flow rate of channel 2, as explained earlier.

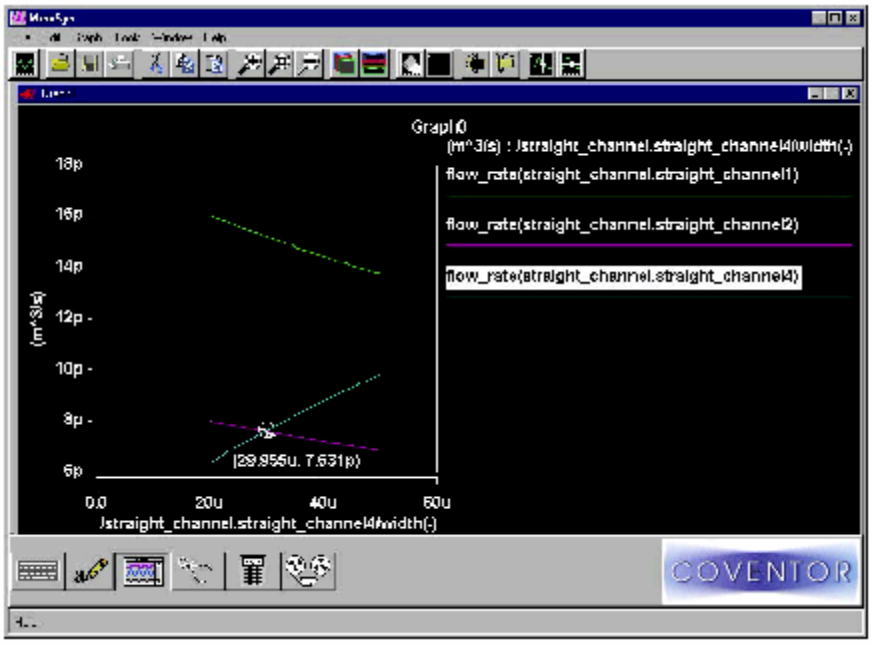


Figure 3-7 MemSys Graphics Window

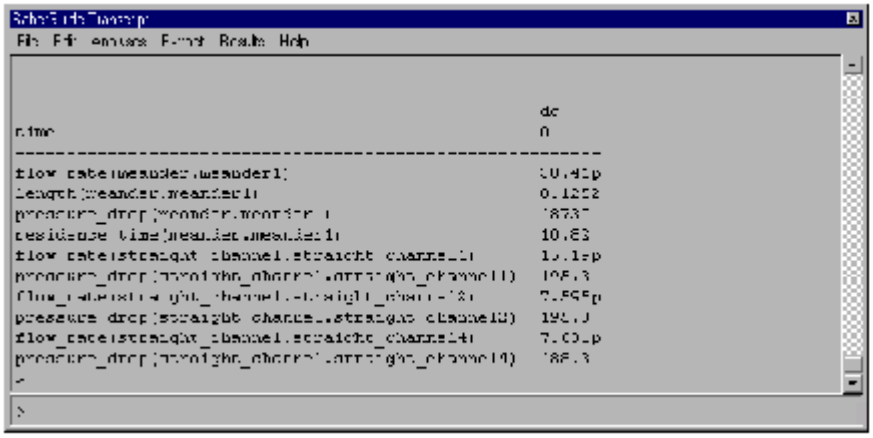
16. In the Saber Guide Transcript window output the data to a text file using **Results > Plotfile Report >Input/Output.** Specify an **Output File Name,** and click **OK**. The file will be stored in the drug_screening\Schematics directory. Close any windows that open.

17. Close the two small results windows and exit from the MemSys graphics window.

3.4: Run Simulation with New Width (Part C)

1. Go back to the MemSys Sketch module and set the width of channel 4 to 29.878 µm by double clicking the channel 4 symbol and typing in the value.

2. Run a DC operating point analysis (refer to Part A for details) and check the result, see Figure 3-8.



Note: Results may vary.

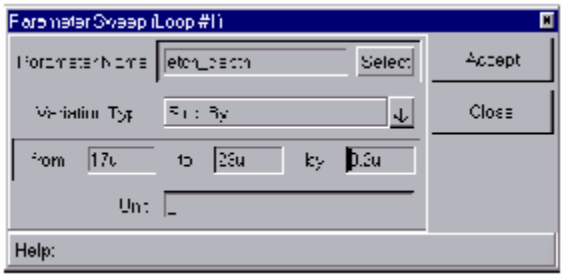
Figure 3-8 Results

3. The flow rate of channels 2 and 4 are now matched, with the flow rate of channel 1 being twice as large. The required mix-ratio is achieved while matching the requirement of a minimal mask width of 10 µm.

3.5: Sensitivity to Process Variations (Part D)

1. The foundry indicated the following specifications of their glass wet etching process:
   Etch depth +/-10%
   Etch uniformity over wafer +/- 5%.

2. Set up a 'Vary' analysis (refer to Part B for details) with the parameters in the following window. Type in the parameter name etch_depth as the variable will not be available from the Select option.



3. Plot the resulting flow rates in one graph (Figure 3-9).

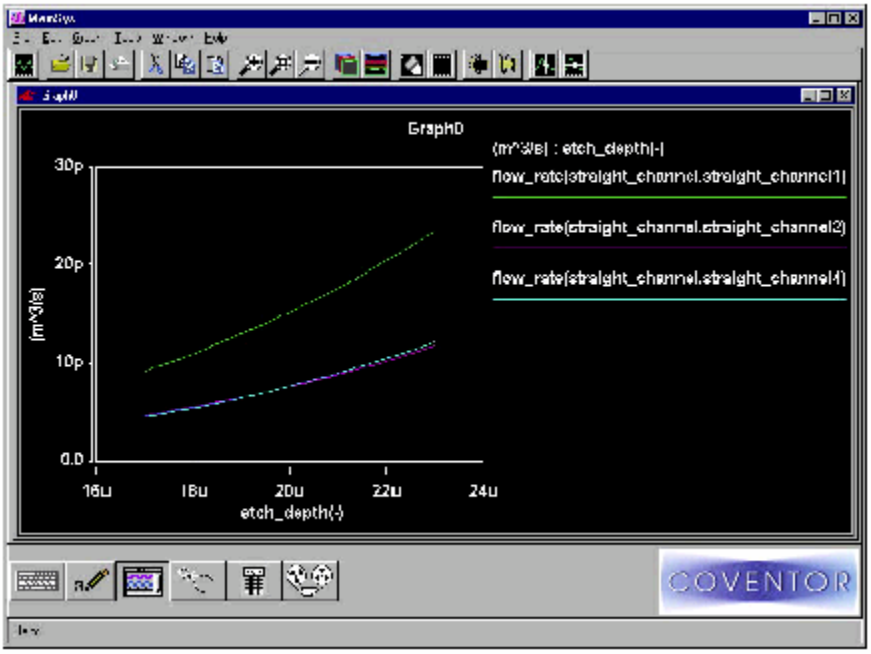


Figure 3-9 Flow Rate Graph

4. To investigate the mix_ratio as a function of overall etch_depth, the signals ‘flow rate channel 4’ and ‘flow rate channel 2’ should be divided using the signal calculator. Click on the *Calculator* icon on the bottom of the screen (Figure 3-10).

Figure 3-10 Calculator

5. Select **flow_rate (straight_channel.straight_channel4)** from the results window (window labeled **design1.sweep**), and copy the signal to the calculator by clicking on the calculator screen with the middle mouse. Repeat this for channel 2.

6. Push the divide **(/)** button to divide both signals.

7. Plot the result by clicking the **Graph X** button at the top left of the calculator (you may need to expand the window), see Figure 3-11. Clear the calculator **(clx)**, and repeat this process to investigate the mix ratio between channel 4 and channel 1.

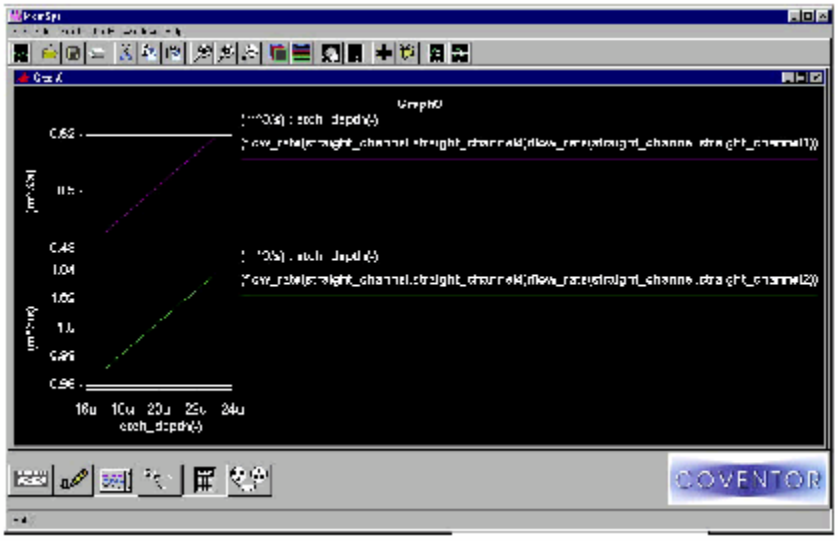
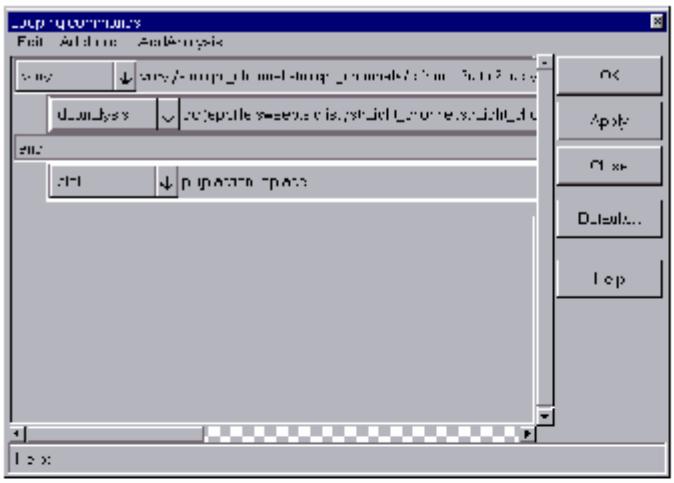
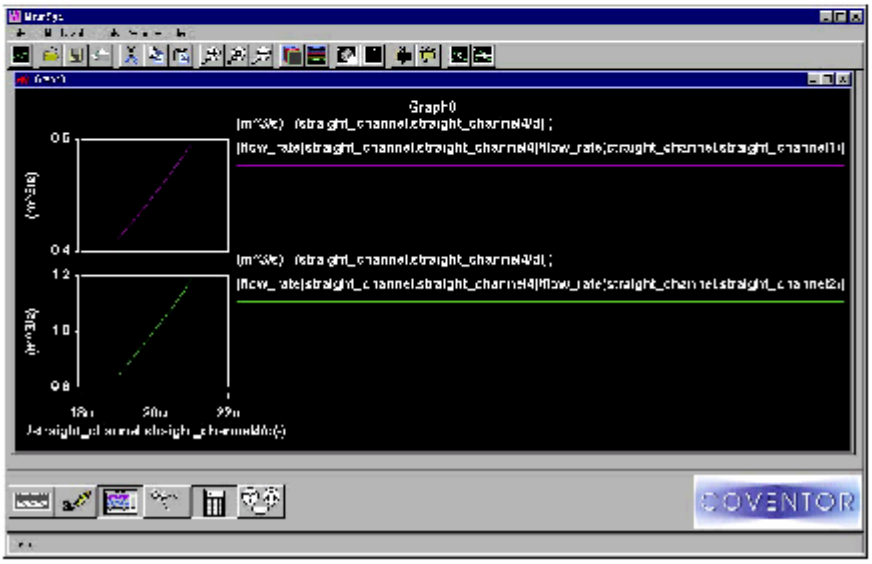


Figure 3-11 Results Window

These graphs reflect the influence of overall etch depth on the mix ratio. The influence on the overall flow rate is negligible.

8. The influence of 5% uniformity can be investigated by varying the depth of a channel and plotting the mix ratios. To do so, set up a 'Vary' analysis and vary the width of the selected channel plus and minus 5% (set "d" from 19u to 21u by 0.5u). In the window below the depth of channel 4 is varied:





This supports the conclusion that the non-uniformity of etch depth has a larger influence on the mix ratio than the tolerance in overall etch depth.

3.6: Conclusions

Typical design issues such as flow rates settings, mixing ratios, and sensitivity analysis can readily be solved by system level fluidic modeling rather than by performing lengthy FEM simulations. A large number of parameters can be varied and the effects studied within seconds, resulting in a better understanding of the system behavior.

Section 4: SwitchSim

4.1: Introduction

Electrokinetic microfluidic microsystems are powerful analytical tools for many applications, such as nucleic acid analysis, enzyme assays, and immunoassays. These systems follow a typical sequence: sample injection, mixing, chemical reaction (modification), separation, and detection. Electrokinetic change is used to transport the specimen through the channel. Complicated relationships exist between the micro channel geometries and the behavior of the multi-component fluids. The SwitchSim module is designed to assist the designer in choosing optimal system settings for the pinch field during injection and for the switching field in a switch component.

The tutorials in this chapter illustrate the steps necessary to analyze a sample injection and switching model. The tutorials contrast the results with and without the introduction of electronically induced constriction of the horizontal channel at the area of intersection. All structures are built within the Coventor software environment and thus do not require any external files. Although the model is simple, such intersections are powerful components that enable one to separate chemical species.

4.1.1: Switching Flow

The species can be separated by switching the electrical field at a channel intersection. The sequence of the switching flow is shown in Figure 4-1 (this figure also shows the voltage setup for Tutorial A). The left figure shows the electrical field at the first phase: an initial Gaussian distribution enters the horizontal channel from the left. The right figure shows the electrical field at the second phase: the electric field is switched in order to drive a segment of species into the transverse (separation) channel.

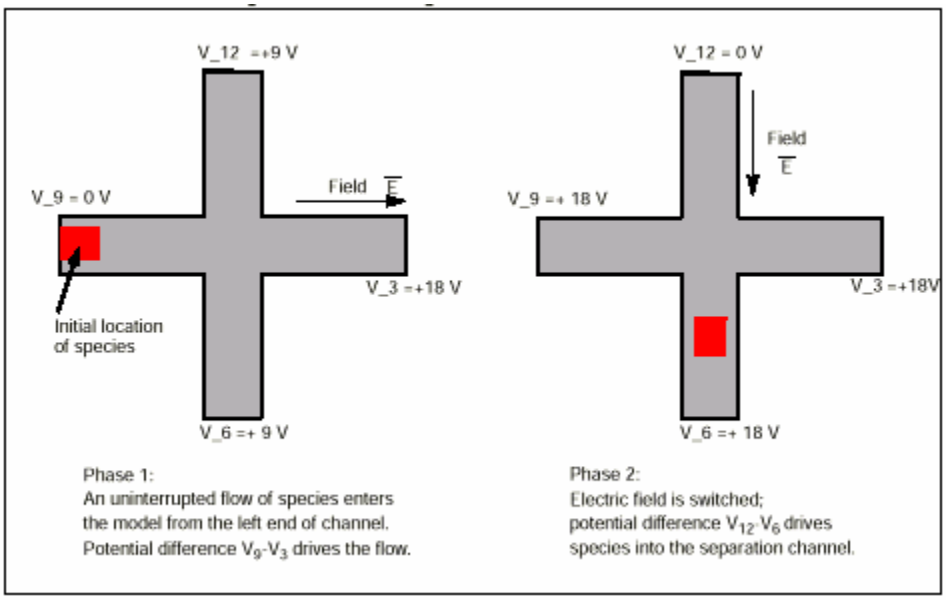


Figure 4-1 Switching flow at channel intersections

4.1.2: Theory

In this brief section, electrophoresis and electroosmosis are introduced in Figure 4-2 and Figure 4-3.

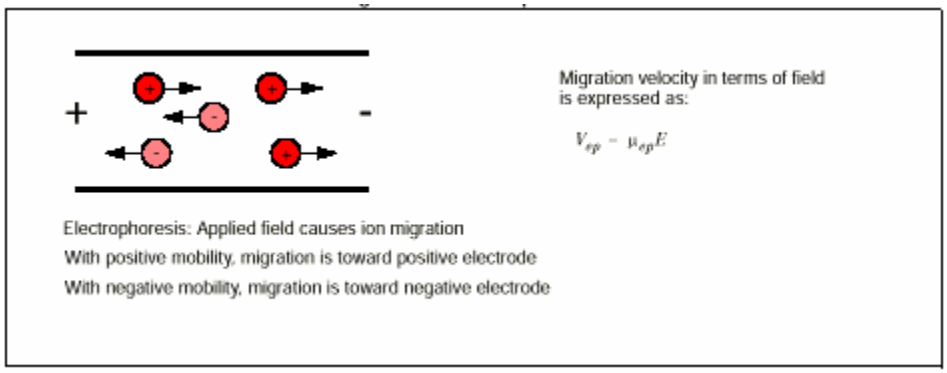


Figure 4-2 Electrophoresis

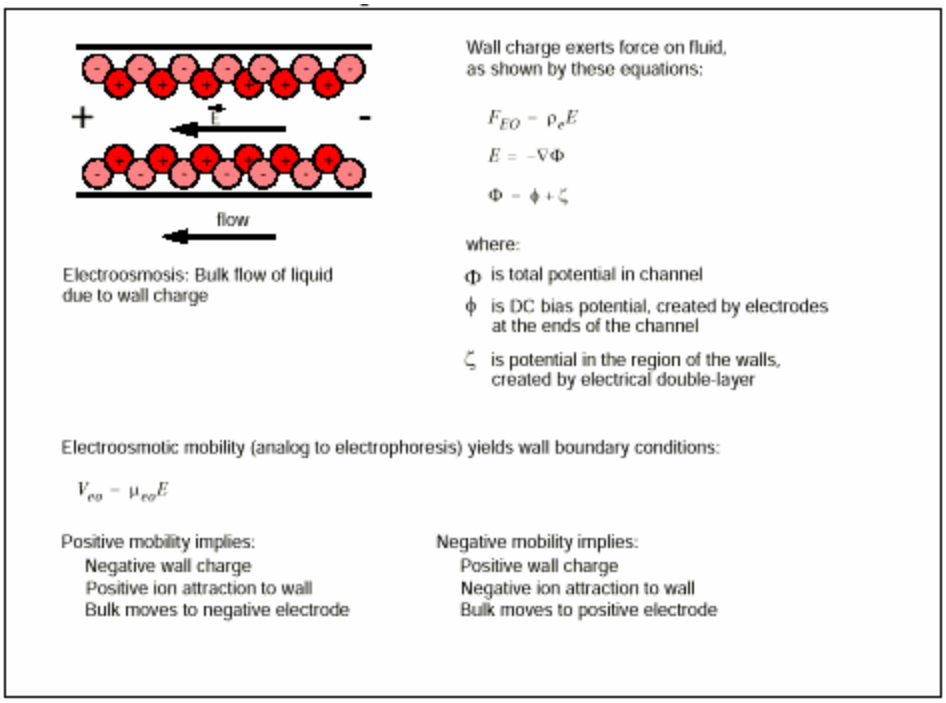


Figure 4-3 Electroosmosis

4.2: Tutorial A

This tutorial simulates injection and unpinched switching, using a simple channel cross. The species input is defined, then boundary conditions are assigned to allow channel switching and controlled species flow. Table, graph, and full 3-D color mapped solutions are viewed, and a variety of output analysis tools are demonstrated using the Visualizer. The channel cross is shown here:

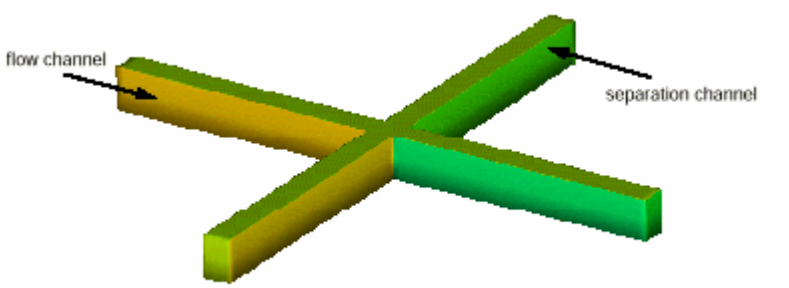
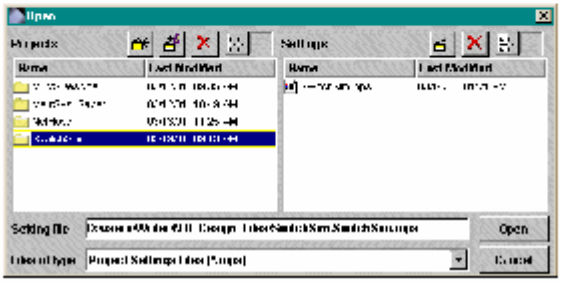


Figure 4-4 Channel model

4.2.1: Initialization

The tutorial starts by launching the software and creating a new project.

Step 1: Launch CoventorWare and import the tutorial	
User	a. Click the desktop icon (UNIX users enter *coventorware*) to start the program. **b.** In the Project window that opens, select the *Import tutorial* icon. **c.** In the new window that appears, select *SwitchSim*. **d.** Click on **Open**. **e.** Click **OK** to close the confirmation box. **f.** In the project dialog window, select the *SwitchSim* directory. A default *.mps* filename will appear in the window. **g.** Click on **Open**.



4.2.2: Material Properties Database

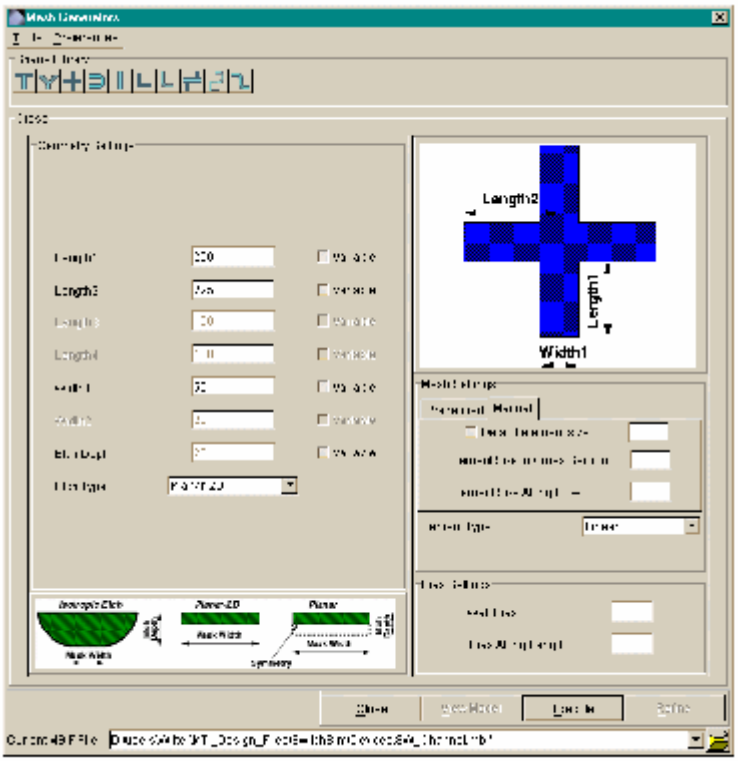
Step 2: Verify path and file	
User	**Explanation**
Select the *Foundry* tab. Ensure that the **Materials** field has a correct path to a valid .mpd file.	The file path and name of the correct .mpd file should appear by default in the *Materials* field. If not, click the folder icon and navigate to the correct .mpd file.

4.2.3: Mesh Generators

Instead of using the Layout Editor and solid model tool, the Mesh Generator tool will be used to design, build, and mesh the device. This tool has built in capabilities for a number of predefined shapes. The geometry and mesh constraints are defined after a general shape type has been chosen from the library. The Layout Editor is used in Tutorial B.

Since the shapes are predefined, it is not necessary to create a .cat file for the layout design. Also, because this tool creates devices for fluidic design, a process file is not needed. The interior is assigned the properties of water as a default. The physical properties for a species within the carrier fluid are defined within a fluidic module.

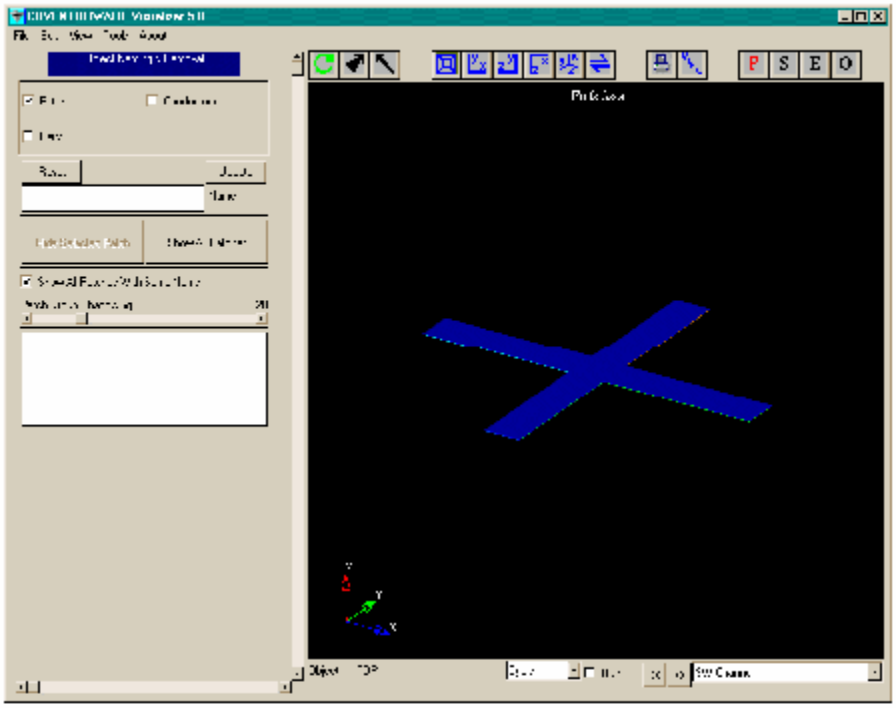
Step 2: Verify path and file	
User	**Explanation**
Select the *Foundry* tab. Ensure that the **Materials** field has a correct path to a valid .mpd file.	The file path and name of the correct .mpd file should appear by default in the *Materials* field. If not, click the folder icon and navigate to the correct .mpd file.


Length2
Length1
Width1

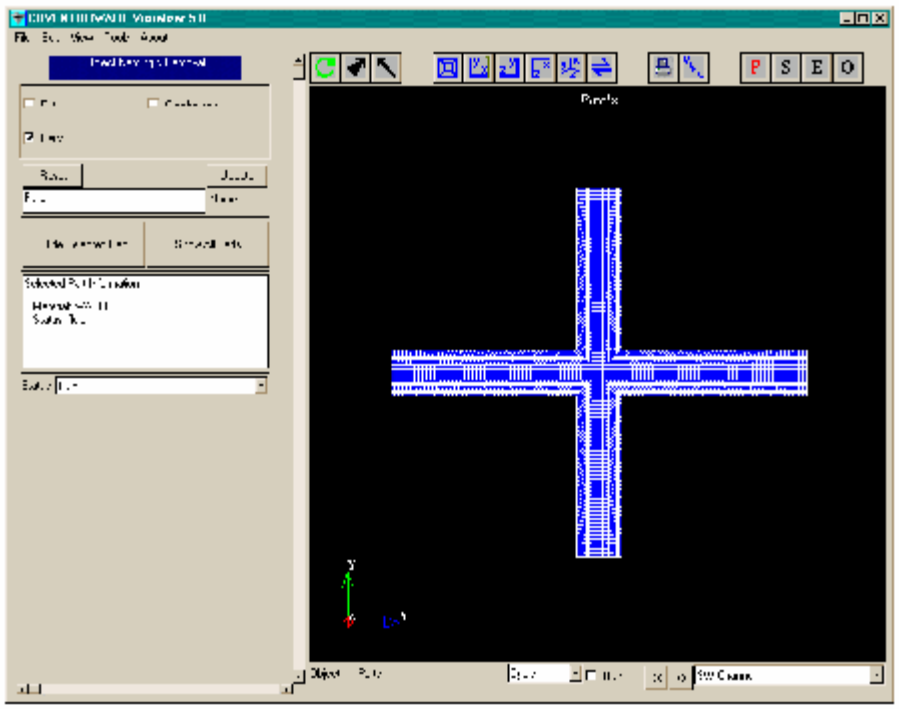
Step 4: Setting model parameters	
User	**Explanation**
a. Set only the fields listed below as described in the Geometry Settings field: Length1 = 200 Length2 = 225 Width = 50 Etch Type = Planar-2D	▬ Larger element sizes will reduce the time necessary to run the simulation, but may result in less accuracy. Conversely, smaller element sizes will create a finer mesh and will also increase run time.
b. Click on the *Manual* tab in the *Mesh Settings* field.	
c. Set the **element size in Cross Sec** = 1	
d. Set the **element size along flow** = 1	
e. Element type defaults to *parabolic*. This must be changed to *Linear*.	
f. *Bias Settings* default values need not be changed.	▬ By default, the file being created will be named *SW_Channel.mbif*.
g. Click **Execute**.	▬ Select **OK** to overwrite, or assign a new name for the file before proceeding.
h. If this tutorial is re-run, the option to overwrite previous results will appear.	

Depending on processor speed, several minutes may transpire before the model is completed and the *View Model* button is activated.

Step 5: View Model	
User	**Explanation**
a. When the Mesh Generator stops running, select **View Model** from the bottom of the window.	**Normalize** zooms to the optimum object size and centers the object in the viewer. **Isometric** gives a view perspective in three dimensions.
b. Select the **Normalize** icon. 	
c. Select the **Isometric** view. 	



Step 6: View Mesh	
User	**Explanation**
a. Check *Parts* in the upper left field of the Visualizer. **b.** Select the **Front View** icon. **c.** Using the middle mouse button, click on the object to display the mesh. **d.** Select **Scale** icon. **e.** Click in the view area and drag upward to zoom in.	If the mesh differs significantly from that shown below, return to Step 3 and review your work.

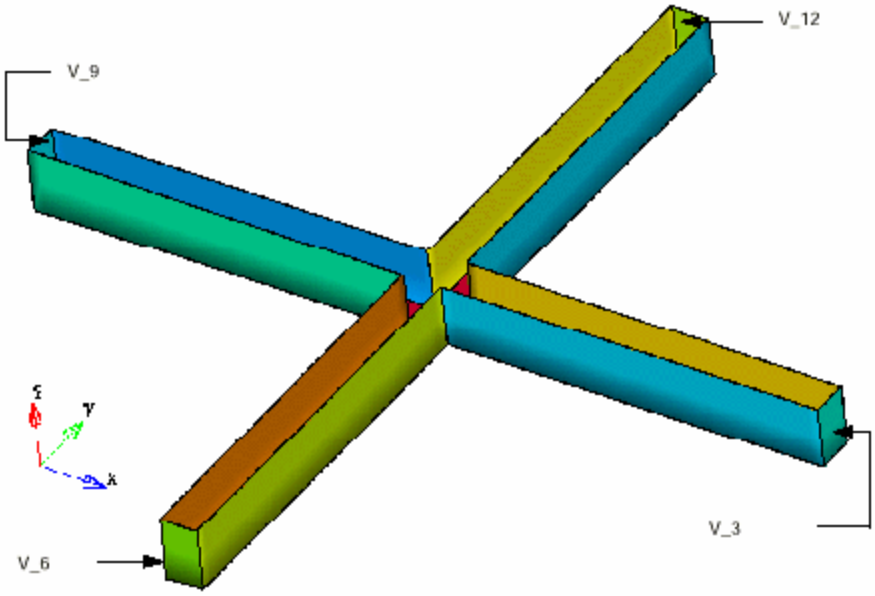


4.2.4: Changing Patch Names

For convenience and clarity, four of the default patch names will be changed.

Step 7: Re-Name Patches	
User	**Explanation**
a. Check *Patches* in the upper left field of the Visualizer. **b.** Using the middle mouse button, click on the object to select the top patch. By default, this patch is designated **patch_0**. **c.** On the left side of the visualizer, click on **Hide Selected Patch**. **d.** Click the icon to change to the **Isometric** view. **e.** Select *Edit > Edit MBIF* from the menu bar. **f.** By default, the Scaling options are displayed. Change the Z Scale value to **50** and click **Update**. **g.** **Close** the Edit MBIF window. **h.** To rename a patch, select it with the middle mouse button, replace the default name with the new name in the *name* field, and click **Update**. Perform these steps for each of the four channel end patches.	The Z scale was increased to make it easier to select the patches on the channel ends. The new names are selected to correspond with clockwise locations.

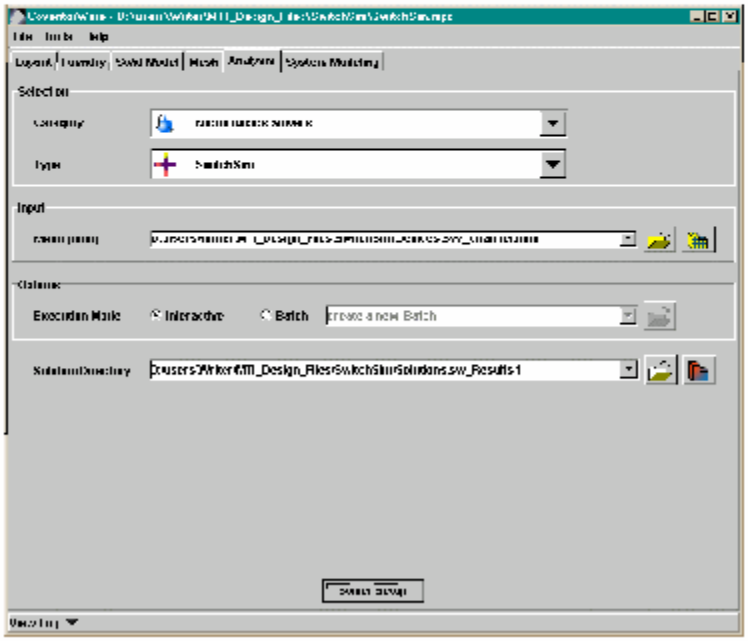
The default patch names that appear in the Visualizer should be changed to those shown here. As long as the XYZ orientation is as shown, the assigned names are correct.



Step 8: Save mbif	
User	**Explanation**
a. Select *File>Save* from the menu bar to preserve your changes. b. Select *File>Quit* to close the Visualizer. c. Click **Close** to close the Mesh Generators window and return to the Function Manager.	It is not necessary to change the Z-scale setting to its original value. Scale adjustments simply modify the presentation, and do not affect the *.mbif* file.

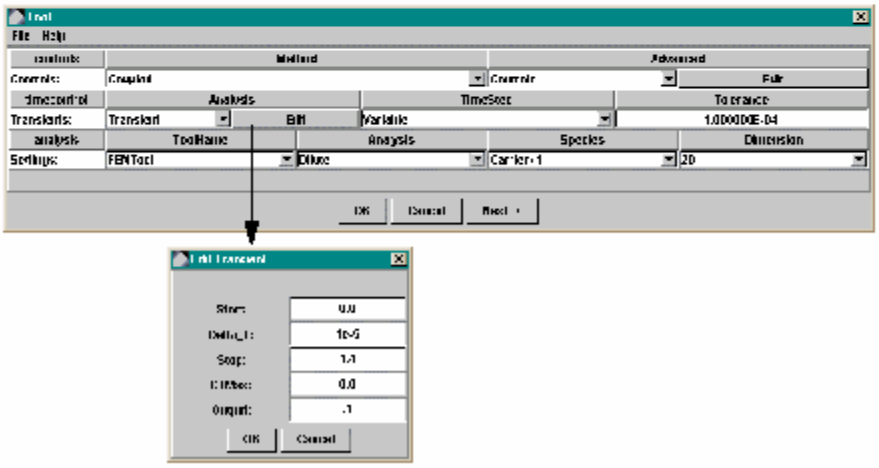
4.2.5: Solver Setup

Step 9: Solver Setup	
User	**Explanation**
a. Select the *Analysis* tab. **b.** In the Category select *Microfluidics Solvers*. **c.** Select *SwitchSim* as the solver Type. **d.** Set the MBIF File path to the *SW_Channel.mbif* file just created. **e.** Set the Solution Directory to *sw_Results1* **f.** Click on **Solver Setup** to open the *Tool* window.	The model type is set for solver use. The Analysis tab settings should match those shown below.



4.2.6: Tool Setup

Step 10: Set Up SwitchSim Tool Window	
User	**Explanation**
a. In the Tool window that opens, set values as shown below. **b.** Select *Edit transient* under *Analysis* in the *timecontrol* field. **c.** Set **Delta_T** to *1e-05* **d.** Set **Stop** to *1.4* **e.** Set **Output** to *.1* **f.** Compare with the view shown below, then click **OK**. **g.** Click **Next** to display the *SwitchSim BCs* panel.	The analysis is transient. The default start time is 0.0 and results will be saved every .1 seconds until the 1.4 second termination. The window is set for transport in a carrier fluid (dilute analysis because carrier fluid predominates). The transient analysis allows the species in this 2D problem to be transported through the switching channels. A series of .mbif files is created to preserve output results obtained for each .1 second step.

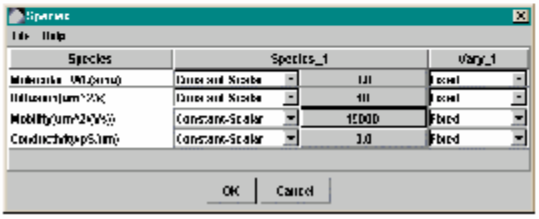


4.2.7: Setting SwitchSim Boundary Conditions

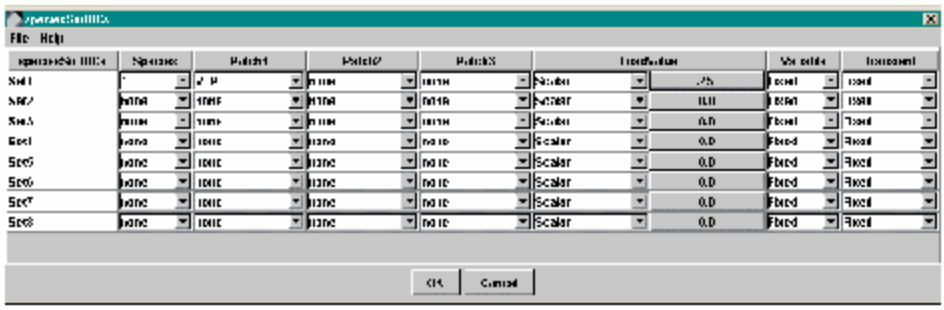
Within SwitchSim, you'll set up the switching boundary conditions for the cross for species injection. "Species" refers to the specimen which is suspended in water within the horizontal channel and is sheared off by the flow of the transverse channel when the voltage is changed.

In this exercise, there are no surface or volume conditions to be set.

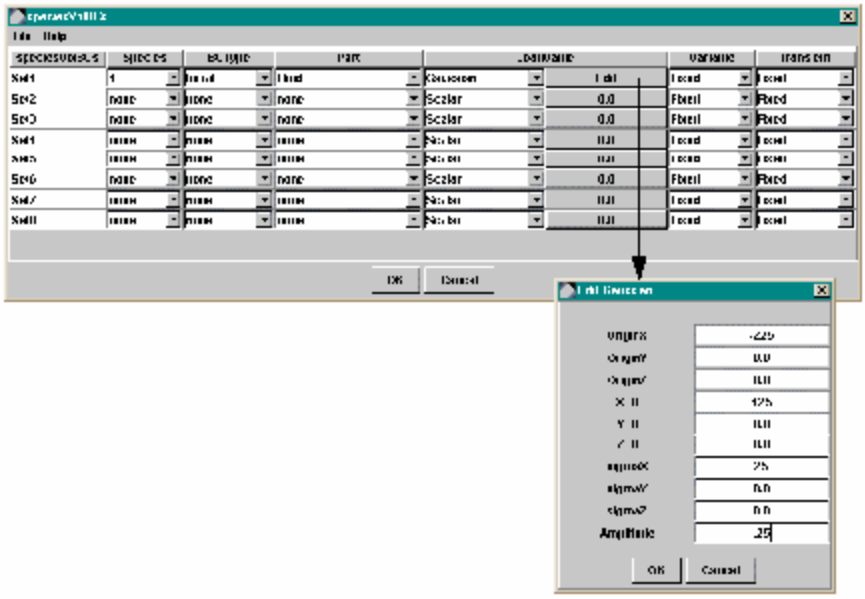
Step 11: Set up SwitchSim Model window	
User	**Explanation**
a. In the SwitchSim BCs window that opens, select the **Species** button. **b.** Set the *Diffusion* value to *30.* **c.** Set the *Mobility* value to *15000.* **d.** Click on **OK**	Molecular weight and conductivity are not factors, and can be ignored. The diffusion and mobility settings are required for accurate simulation of the species transport.



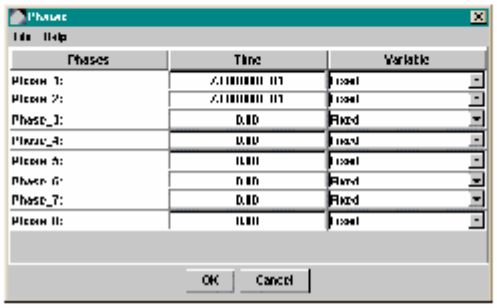
Step 12: Set Species Surface Boundary Conditions	
User	**Explanation**
a. Click on **speciesSurfBCs** **b.** Assign a load value of *.25* for Species 1 at patch V_9. **c.** Click on **OK**	There is only 1 species in this simulation. Patch V_9 is assigned a concentration of .25 to allow a continuous inflow of species from that location.



Step 13: Set Species Volume Boundary Conditions	
User	**Explanation**
a. Click on **speciesVolBCs** button. Enter the following Set 1 values: **b.** Set *Species* to *1.* **c.** Set *BCType* to *Initial.* **d.** Set *Part* to *Fluid.* **e.** Set et *LoadValue* to *Gaussian.* **f.** Set the following Gaussian values: Origin X = *-225* X_0 = *125* sigma X = *25* Amplitude = *.25* **g.** Click **OK** to close the *Edit Gaussian* dialog box. **h.** Click **OK** to close the *speciesVolBCs* window.	The precision of the volume boundary conditions defines the initial location of the species within the channel. A flat top Gaussian distribution with a center point at x=-225 microns and a sigma of 25 microns is specified in order to provide an initially smooth species concentration profile. This is not only a more realistic initial condition than a step function change in species concentration, it also allows for a numerically more accurate result.



Step 14: Set Phase parameters	
User	**Explanation**
a. Select *Phases* from the SwitchSim BCs control panel. **b.** Set the time value for Phase_1 to 0.7 (7.000000E-01). **c.** Set the same value for Phase_2. **d.** Click **OK** to close the *Phases* dialog box.	The phases are periods of time during which specified voltage conditions prevail.

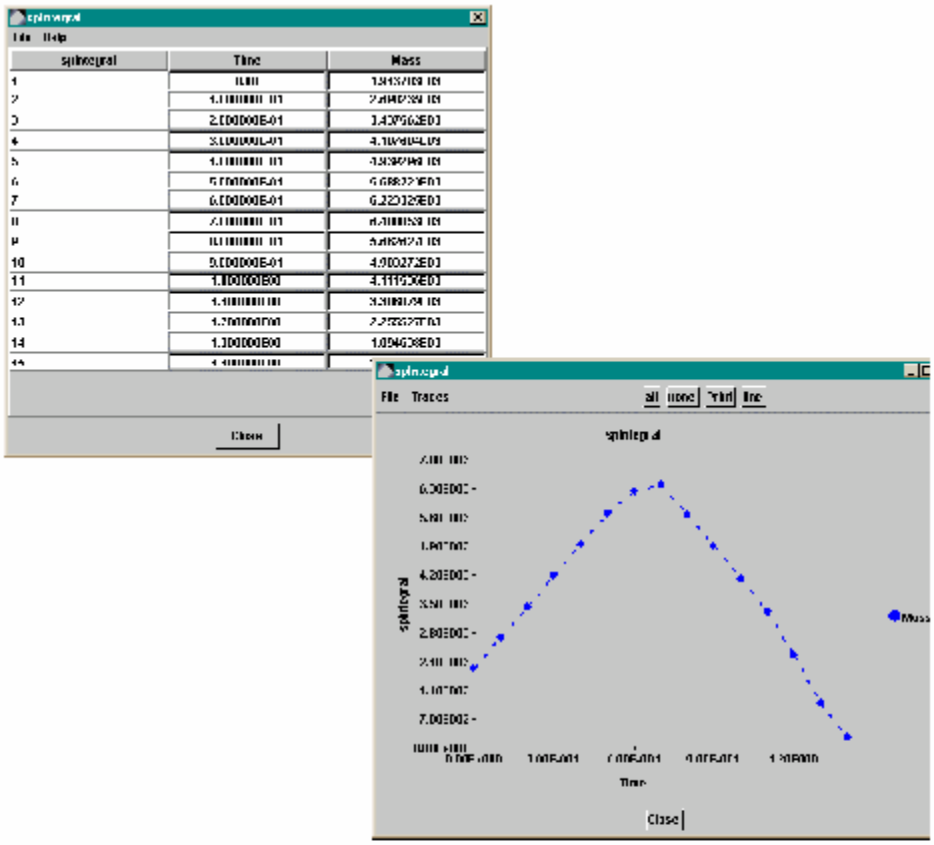


Step 15: Set Switch Boundary Conditions	
User	**Explanation**
a. Select **SwitchBCs** from the SwitchSim BCs control panel. **b.** Set the first four ports as illustrated below. **c.** Edit the Phase voltages according to these settings: **d.** Click **OK** to close each *Edit Phase Voltage* dialog box after entering the correct values. **e.** Click **OK** to close the SwitchBCs dialog box. **f.** Click **Simulate**. **g.** When prompted to save settings, select **Yes**.	The patches at the ends of each channel are ports used to control voltage changes during the simulation. The phase table sets the voltage values that will exist during each phase. During phase 1, mass increases as species enters the system from the left port (V_9). At time 0.7 (phase 2) the mass begins to decrease as species leaves the system. Simulation times vary depending on processor speed, but will take at least 5 minutes.

	Patch	Phase 1	Phase 2
Port 1	V_12	9	0
Port 2	V_3	18	18
Port 3	V_6	9	18
Port 4	V_9	0	18

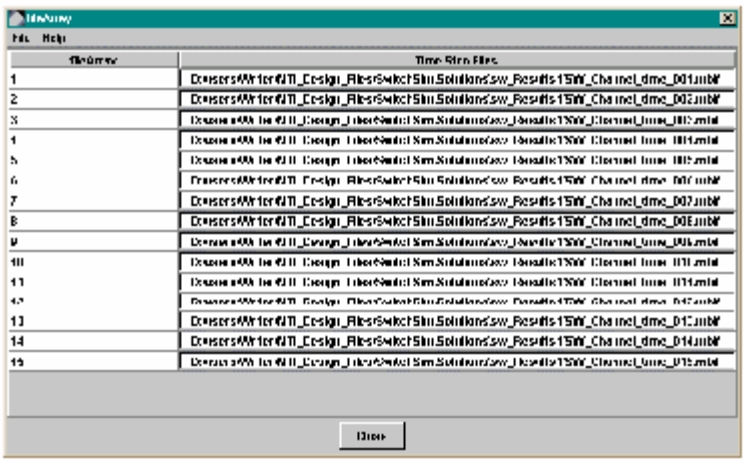
4.2.8: Simulation Results

Step 16: View the SwitchSim table results	
User	**Explanation**
a. In the Simulation Results window that opens, click on **spintegralTable**. **b.** Click on **Close** after viewing results. **c.** Click on **spintegralGraph**. **d.** Click on **Close** after viewing results.	The windows show the results of a conservation of mass of the additional species, with a calculation at each time step specified in the SwitchSim Tool window. As the species moves from left to right in the channel, some of the mass of the additional species exits accounting for the observed trend. Plugs of species leave the model because they are electrokinetically driven out: diffusion is responsible for only a small portion of the mass that leaves the model.



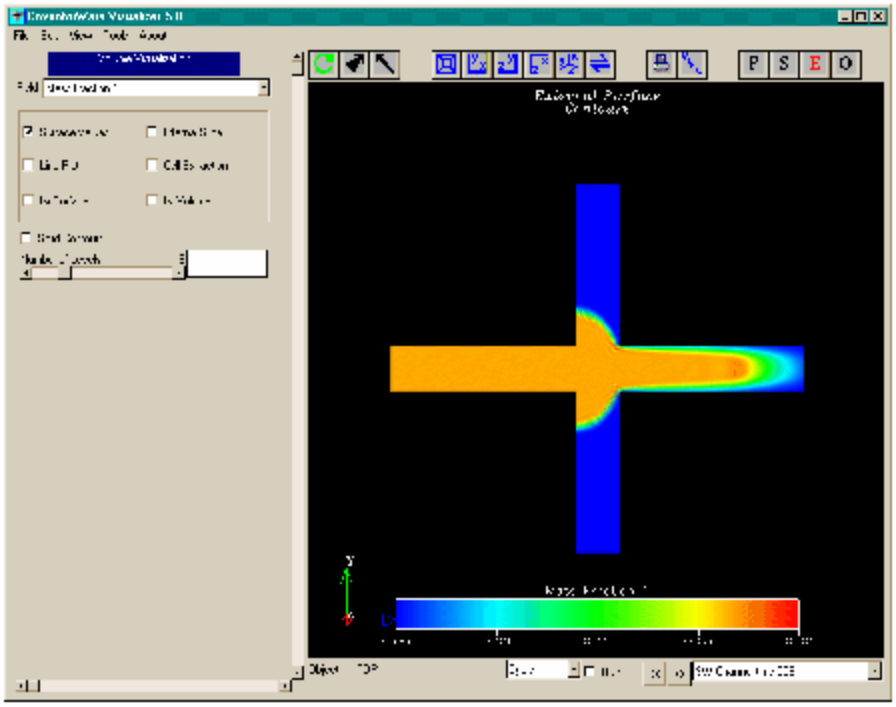
The value of the mass remaining in the channels may vary from the depicted table values below, especially by the end of the simulation. Residual numerical errors are responsible for the difference. These errors depend primarily on the computer used and should be within 5% as reported.

Step 17: View the List of Time Step Files	
User	**Explanation**
a. Click on **fileArray**. b. Observe the names and file paths of the 15 .mbif files created during the simulation. c. Click on **Close**.	The window lists the mbif files retained during the calculation. Because they were saved, they can be viewed with the Visualizer.

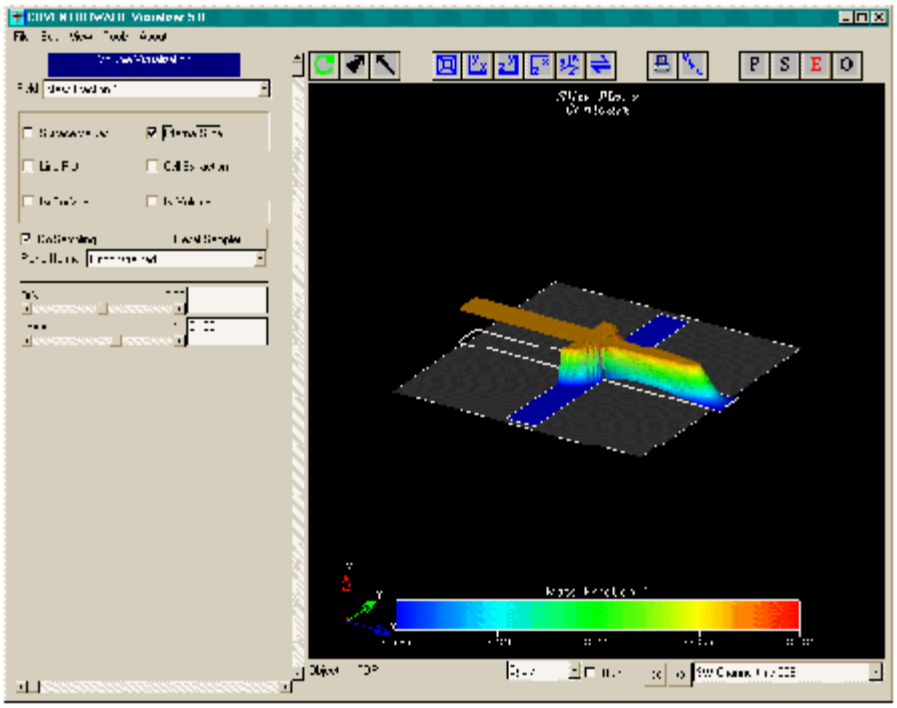


Step 18: Start the Visualizer	
User	**Explanation**
a. From the Visualizer Control Panel menu bar window, click on **Start Visualizer**. **b.** Click on **Visualize List**. **c.** Set the **Isometric View** orientation and **Normalize** the view. **d.** Click the E icon (*Volume Visualization*) on the Visualizer toolbar.	The Visualizer can display all the mbif file results.

Step 19: Set up the Visualizer for Mass Fraction results	
User	**Explanation**
a. From the Visualizer menu bar, select *Edit > Edit MBIF.* **b.** Select the *Active Fields* check box. **c.** Uncheck the *Mises* and *Displacement* Volume fields. **d.** Check the *Mass Fraction 1* field. **e.** **Update** and **Close** the window. **f.** Click the *Front View* (yx) button on the Visualizer toolbar. **g.** Use the >> button at the bottom to advance through the solution steps to *SW Channel time 006*. Compare with the view shown below. **h.** Check the *Run* option to observe the animated simulation.	The control settings enable viewing the movement of the species.



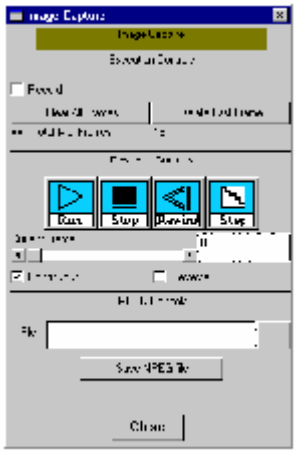
Step 20: Set up the Visualizer for internal slice plane results	
User	**Explanation**
a. Click on **Isometric View** from the Visualizer toolbar and adjust for magnification. **b.** From the Visualizer left panel, click on *Internal Slice*. **c.** Check that the Offset slider is set to *0* and that the Scale slider is set to *0.1*. **d.** Along the menu bar, select *Edit > Edit MBIF* and check *scaling*. **e.** Set the Z Scale to *50*. **f.** **Update** and **Close** the Edit MBIF window. **g.** Along the top of the Visualizer main window, click on the **View** icon to edit the view. **h.** Verify that the Transparency slider is set at *1.0*. **i.** **Close** the General Editor window. **j.** Advance through the solution steps manually, or check the *Run* box for animation.	The slice view allows display of the Mass Fraction magnitude at the center of the channel. The plug moves down the channel. You can observe the effects of diffusion with time. A selected event time is shown below.



4.2.9: Animated Files

MPEG files are a convenient way to save or transport graphical representations of simulation results. MPEG files can be created through the Visualizer. These files can be played on standard Windows media players.

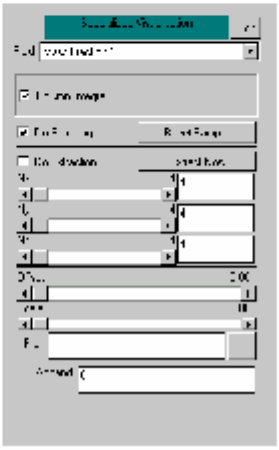
Step 21: To Capture the Sequence as an MPEG Animation	
User	**Explanation**
a. From the menu bar, select *View>View Editors>View Editor* to open the View Editor. Open the Resolution drop-down menu and select any of the four numerical options, depending on the screen size desired for playback. **Close** the editor. **b.** Set the Visualizer time step in the lower right corner to *SW Channel time 015*. **c.** From the menu bar, select *Tools>Image Capture*. **d.** In the Image Capture window (shown below), check *Record*. **e.** Use the controls at the bottom of the Visualizer window to step through the sequence of images. **f.** When all images in the sequence have been viewed, uncheck *Record*. **g.** Select **Rewind**. **h.** Check the *Continuous* option. **i.** Select **Run**. **j.** Click on the icon to the right of the *File* field to open the *fileDialog* dialog box. Provide a name for the MPEG animation and click **OK** to close the box. Observe the path and file name in the Image Capture dialog box. **k.** Click **Save MPEG file** to create the file and **Close** to close the dialog box.	Before creating the animation, it is necessary to change the resolution setting. By default, the Visualizer resolution is set to *Full View*. This must be set to a numerical value that can be interpreted by the media player. The series of .mbif files appears temporarily in the *log* directory, but is automatically deleted when the MPEG file is compiled. When the number of old logs exceeds 4, the system will prompt for the deletion of old logs at start-up. Remember to move or copy the completed MPEG before deleting old logs.



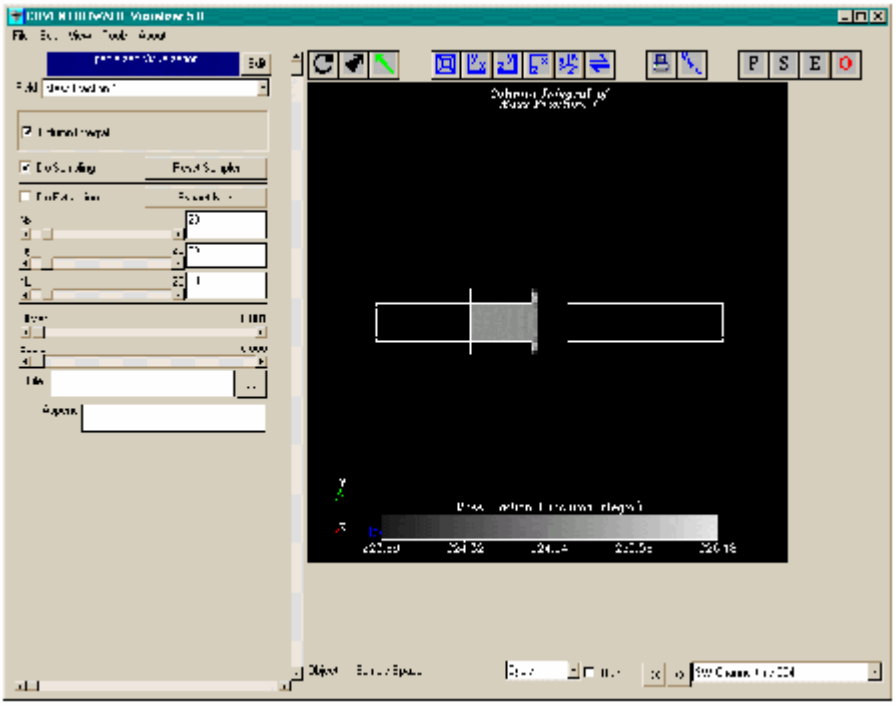
4.2.10: Column Integral Results

Step 22: Set up for column integral results	
User	**Explanation**
a. Click on the **O** icon (*Specialized Visualization*) to the far right of the Visualizer window. **b.** In the control panel that opens on the left, click the **Edit** button in the upper right corner. **c.** In the window that opens, check *Column Integral*, then **Close** the window.	This technique is used to analyze the species concentration at a specific point in the channel.

The Techniques window and panel are shown here:



Step 23: Set up for column integral results	
User	**Explanation**
a. Along the top window, click on the **Front View** (*yx*) icon. **b.** In the main display, click with the middle mouse button on the cube outline. **c.** Along the top window, click on the **Scale**  icon. **d.** Click on the cube boundary; reduce it to be about 25% larger than the channel width. **e.** Along the top window, click on the **Translate**  icon. **f.** Click on the cube boundary and move it along the channel. **g.** In the lower right corner of the main window, select *SW_Channel time 004*. **h.** Along the top window, click back and forth on the **E** and **O** icons. Continue until you can position the cube to where most of the species is located. **i.** Each time you toggle back to **O** mode, middle mouse click on the cube to select it. **j.** In the left panel, move the Nx, Ny and Nz sliders to a value of *20*. **k.** Next to the File field, click on the ... icon and set the file name to *column.txt*. **l.** Click on **Extract Now**.	▪ The column integration technique allows you to emulate the measurement of species concentration. The extraction process creates data that projects a surface plot over the channel. The intensity of the plot shows the species concentration in that location. ▪ The Nx, Ny, and Nz sliders represent the number of boxes in the large bounding cube, across which the integration and extraction are to be performed. ▪ The values obtained depend on the size and location of the cube. Figure F4-5 shows sample results.



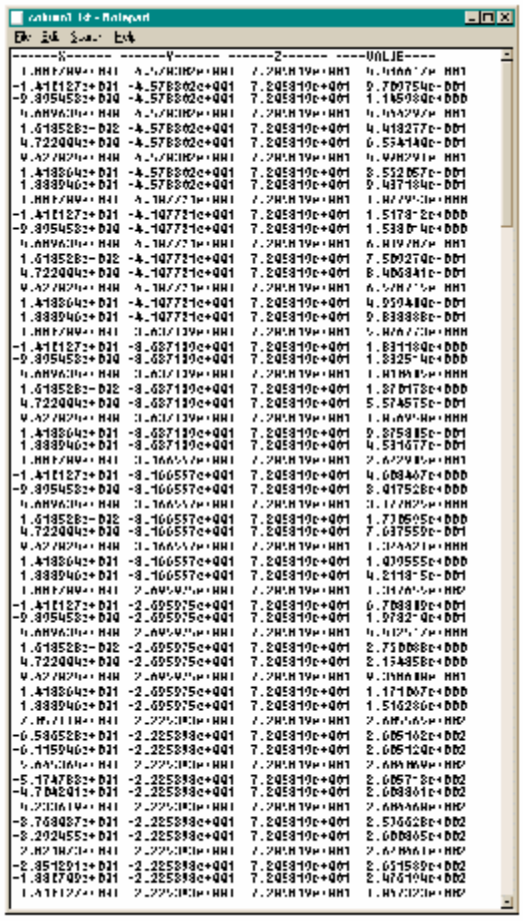
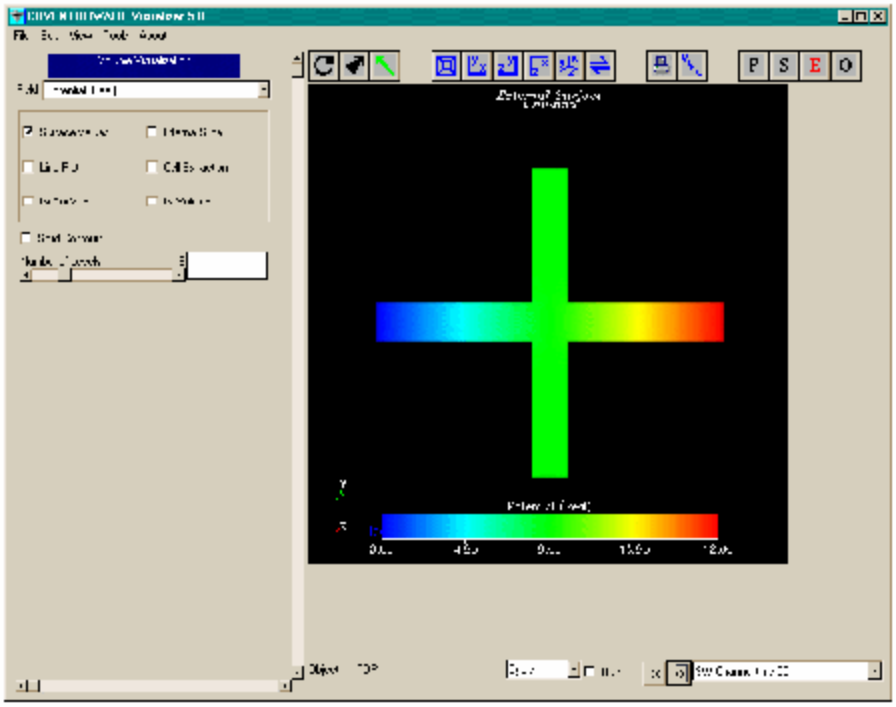
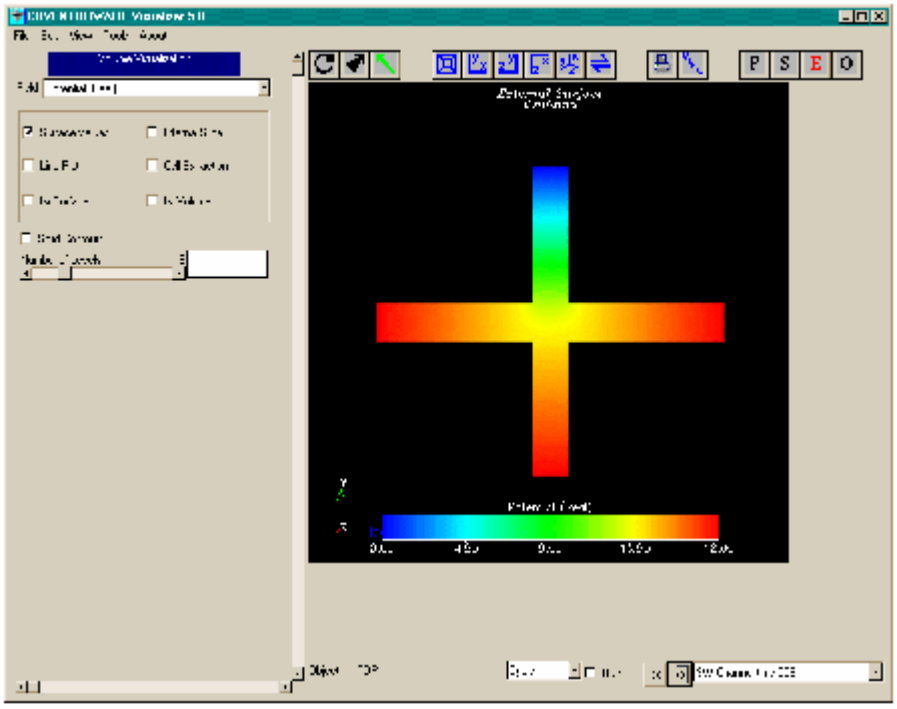


Figure 4-5: Sample of File Results

Step 24: Set up for potential results	
User	**Explanation**
a. Along the menu bar, select *Edit* > *Edit MBIF*. **b.** Change the Upper Percentage Offset to *100*. **c.** Click on **Update**. **d.** Click on *Active Fields*. **e.** Scroll down and enable *Potential*. Disable any other active fields. **f.** **Update** and **Close** the Edit MBIF window. **g.** Along the top of the main window, click on the **E** (*Volume Visualization*) icon. **h.** From the Visualizer left panel, click on *Surface Values*. **i.** Select the *Run* check box to automatically advance through the solution steps. **j.** When finished, **Stop Visualizer**. **k.** Click on **Done** to close the hierarchical results window.	Notice that only the *SW_Channel_time_001.mbif* and *SW_Channel_time_009.mbf* show non-zero potential distribution. This is an intentional space-saving technique, where only the first mbif stored after switching retains the new potential distribution.





Special note about the storage of steady state results

SwitchSim transient simulation solution files store steady state results (such as velocity, pressure, voltage, and current density) in only the first transient mbif file after switching. All fields that change with time (such as mass fractions) are visible in all mbif files.

As an additional exercise, the user can pinch the flow by changing the switchBC's to:

Port	Phase 1	Phase 2	
V_12	0	0	(unpinched Phase 1 value is 9)
V_3	18	18	(same values as unpinched simulation)
V_6	0	18	(unpinched Phase 1 value is 9)
V_9	0	18	(same values as unpinched simulation)

and then rerunning the problem. These values are used in Tutorial B.

If less than 256 Mb of RAM are available, change the Tool parameters so that the post_analysis Output Edit window is set for *0.5* instead of *0.2*.

4.3: Tutorial B

The templates in the shape library offer convenience at the expense of flexibility. In the tutorial just completed, linear variation of the model is possible, but curved, tapered, flared, or angled channels cannot be created. If a more complex channel configurations is desired, it must be built using the Layout Editor.

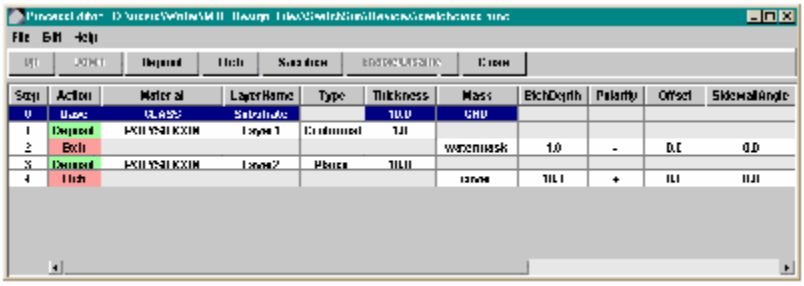
In this tutorial, the T-shaped separator will be created and the capability of constructing channels with virtually any desired geometry will be explored. The resulting model will be meshed and the horizontal channel will be electronically constricted by changing the switchBC values. Finally, the simulation results will be compared with those obtained in the previous exercise.

Step 1: Launch CoventorWare	
User	**a.** Start CoventorWare if it is not running. **b.** Select SwitchSim and enter *crossdesign.mps* as the name of the Setting file.

4.3.1: Review Foundry Process File

Typically, a foundry has a process file which is included with its Design Kit. This file defines the chronology of deposit and etch steps used in the fabrication process. The names of the layers used when building the model must be the same as the mask names given in the process file.

Step 2: Obtain mask names from process file	
User	**Explanation**
a. Select the *Foundry* tab. **b.** Navigate to the *switchcross.proc* process file. **c.** Start the Process Editor.	Observe the mask names used in this process. These masks will have to be created in the Layer browser.



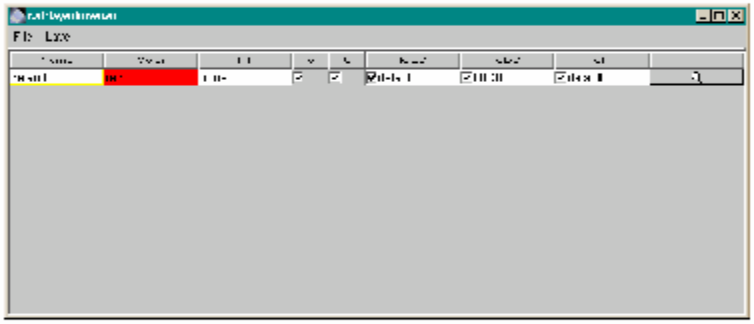
Notice the polarity of the first etch. The shape etched into the first deposited layer is defined by this mask, and will be a cavity with a depth of 1 micron. Positive polarity would result in the removal of all of Layer1 except the portion covered by the mask.

Layer2 encloses the channel and is not etched.

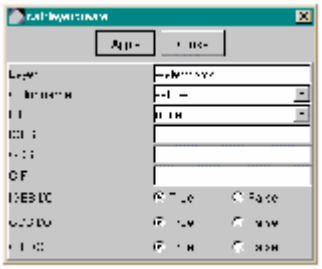
4.3.2: Create Necessary Layers (Masks)

Step 3 : Open the Layer browser	
User 	**a.** **Close** the Process Editor. **b.** Select the Layout tab. **c.** Click the *Start Layout Editor* icon. **d.** Click the *Layer browser* icon.

In this exercise, the Layout Editor starts with just a default layer.

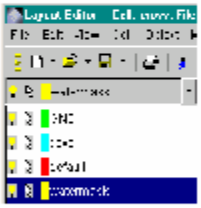


Step 4: Create new layers	
User	**Explanation**
a. Select *Layer > New* **b.** Create a yellow layer named *watermask*. Click **Apply**. **c.** Create a green layer named *GND*. Click **Apply**. **d.** Create a cyan layer named *cover*. Click **Apply**.	The particular colors are not necessary for an accurate simulation, but are given so results are visually consistent with those shown in this tutorial.

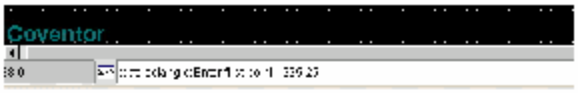


4.3.3: Construct 2-D Channel Layout

Step 5: Change Active Layer	
User	**Explanation**
a. Click **Close** after the third layer is created. **b.** Select *File* > *Close* to close the layer browser. **c.** Open *Current layer* drop-down menu to observe new layers. **d.** Select the *watermask* layer.	If the masks (layers) do not appear as shown here, return to Step 2 and review.

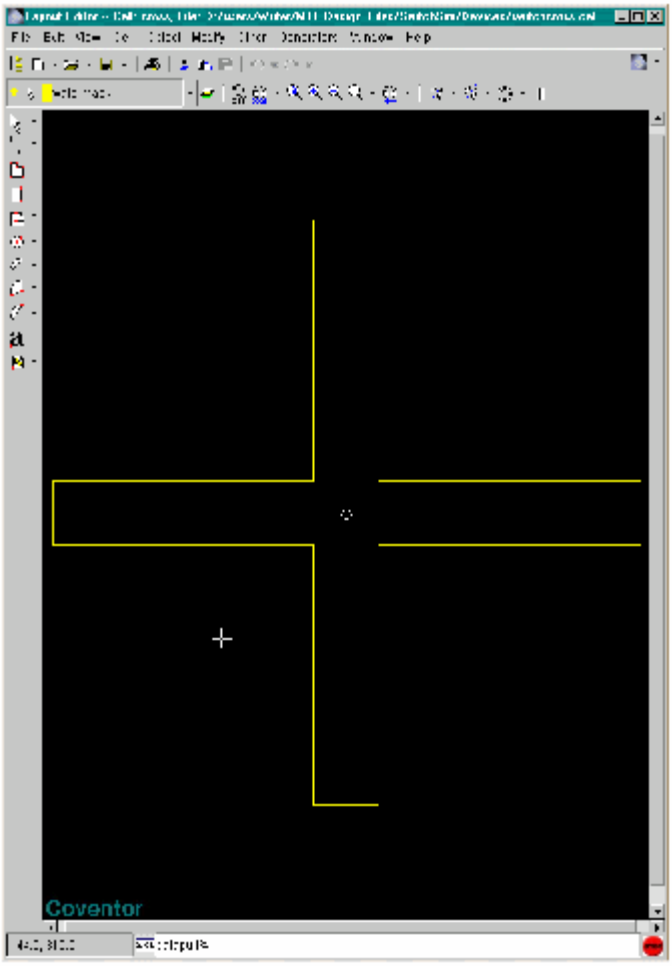


Step 6: Begin construction	
User	**Explanation**
a. Select the *Rectangle* icon from the vertical toolbar. **b.** In the command line, enter the coordinate points *-225 25* as shown.	Rectangles are defined by the coordinates of their opposite corners. Points can be entered either by mouse clicks or by entering the coordinates.



Step 7: Complete rectangles and adjust view	
User	**Explanation**
a. Enter the coordinates *225 -25* in the Command line as prompted to complete the first rectangle. **b.** Build a second rectangle in the same way, using the points (*-25 225*) and (*25 -225*). **c.** Select the *View all* icon.	Selecting *View all* causes the view to zoom out and center.

If an object is inadvertently placed on the wrong layer, or a point coordinate is incorrect, select *Modify* > *Object* from the menu bar and then select the misplaced object. In the dialog box that opens, make the desired corrections and then click **Apply**.



If angled, tapered or otherwise non-orthogonal changes to the channels are desired, those changes are most easily made at this point.

Step 8: Demonstrate edge movement	
User	**Explanation**
a. Select *All angle input*. **b.** From the menu bar, select *Modify > move edge*. **c.** Select the horizontal rectangle. **d.** Select the left edge. Move the edge right or left, then click to re-anchor the edge at a new location. **e.** Click the *Undo* icon to restore the original dimensions.	The *All angle input* icon is above the *Rectangle* icon, and offers two options from its drop-down menu. This demonstration is included to show a tool capability. If more than one change is made, make sure each change is undone.

Step 9: Demonstrate point movement	
User	**Explanation**
a. From the menu bar, select *Modify > move point*. **b.** Select the vertical rectangle. **c.** Select the upper right vertex. **d.** Move the point and observe the changes. Click to anchor the point. **e.** Click the *Undo* icon to restore the original dimensions.	Select the drop-down menu on the *Undo* toolbar icon and ensure all changes have been undone, or delete both rectangles and repeat Steps 6 and 7.

The procedure for creating curved surfaces is more complex and is beyond the scope of this tutorial. The mesh used in this tutorial will not work with curved surfaces.

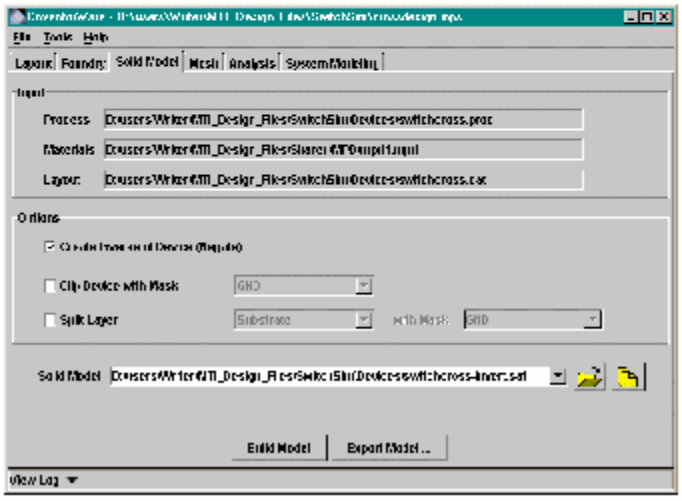
Step 10: Combine rectangles to create a polygon	
User	**Explanation**
a. Select *Modify > Boolean > or* from the menu bar. **b.** Select the rectangles in any order. **c.** Observe the change when the second rectangle is selected.	Since both rectangles reside on the same layer, the order of selection will not affect the result.

The Layout Editor recognizes the resulting shape as a polygon. There are several ways to create the cross. This way was selected because it is straightforward and because it demonstrates the Boolean functionality. Another option is to select the Polygon icon and either point and click on vertices on the canvas, or sequentially enter the vertices in the Command Line.

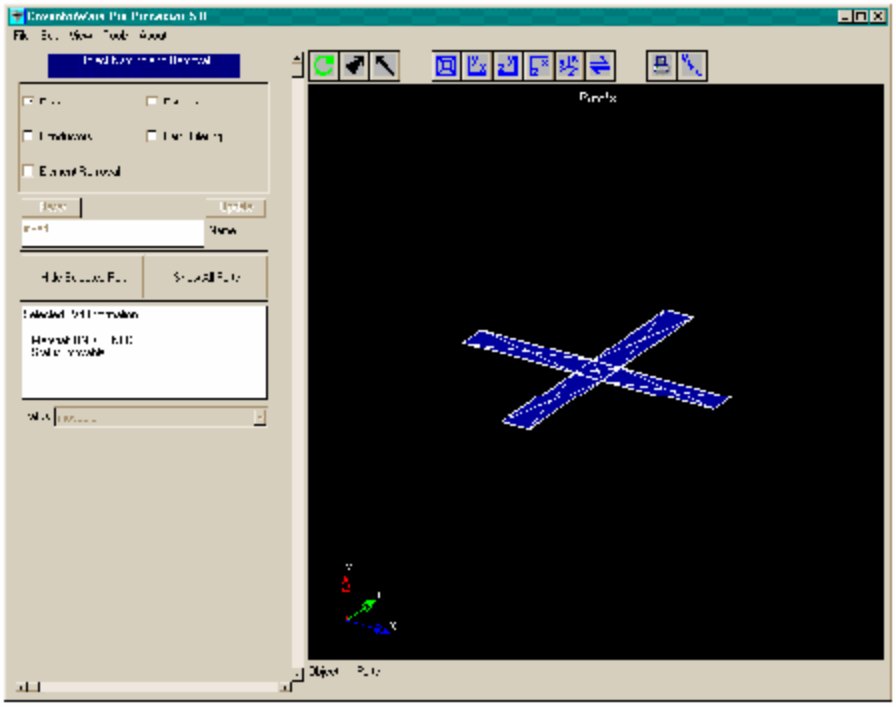
Step 11: Save cell and library	
User	**Explanation**
a. Select *Cell > save* from the menu bar and name the cell *cross*. **b.** Select *File > save* and name the library *switchcross.cat*. **c.** Return to the Function Manager and observe the new path and file name in the *Layout* field, and that the cell name *cross* appears in the topcell field. **d.** Select the *Solid Model* tab.	These steps preserve the two-dimensional model and identify it to the Solid model builder.

4.3.4: Build 3-D Model

Step 12: Set Options	
User	**Explanation**
a. Check the **Create Inverse of Device (Negate)** option. **b.** Observe that the file being created will be named *Switchcross_invert.sat*. This file name will appear by default in the *Solid Model* field.	By selecting the *Create Inverse* option, an object in the form of the model cavity is generated.

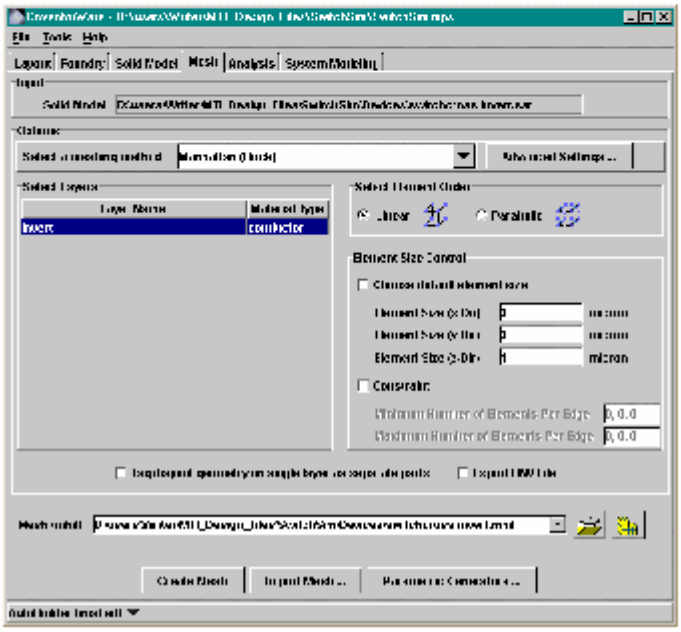


Step 13: Build and view 3-D model	
User	**Explanation**
a. Click on **Build Model**. **b.** When the Visualizer opens, select *isometric view*. **c.** Middle-click on the object to select it and display its properties. **d.** Select *File > quit* to close the Visualizer. **e.** Return to the Layout Editor and select *File > exit*.	Observe the default name *invert* for the object, and notice the material and status. If the model does not appear, check to make sure the layers created match the mask names in the process file, and that the top cell name appears in the Top Cell field on the Layout tab.

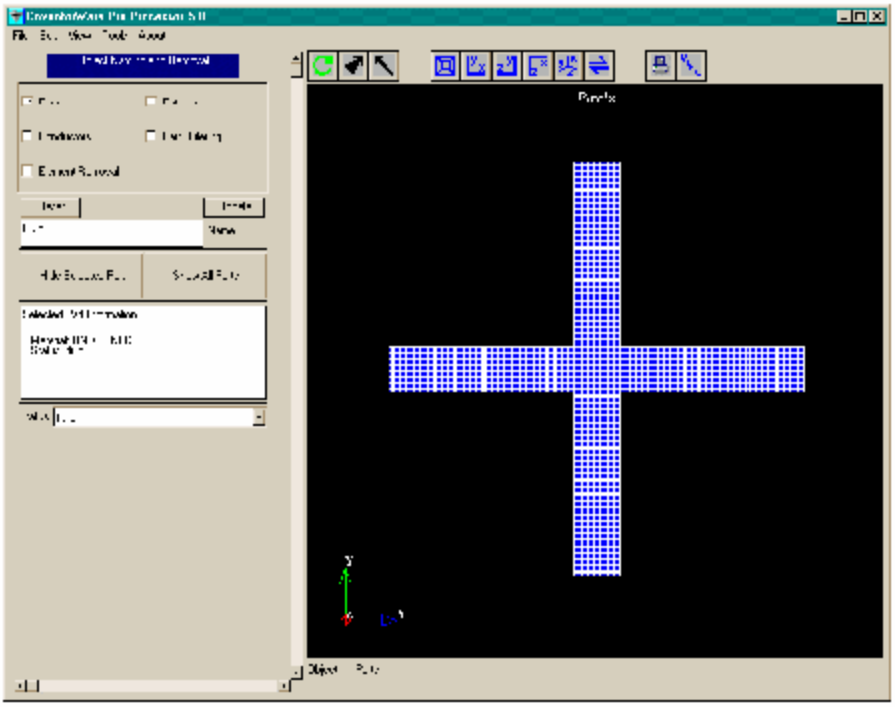


4.3.5: Create Mesh

Step 14: Set mesh parameters	
User	**Explanation**
a. Select the *Mesh* tab and clear the warning box. **b.** Under *Options*, select the *Manhattan (brick)* meshing method. **c.** **Advance settings** default settings are satisfactory for this exercise. **d.** Select the *Linear* element order. **e.** Under *Element size control*, uncheck the *Choose default element size* box and enter *3* for both the X-Dir and Y-Dir element sizes. **f.** Enter *1* for the Z-Dir element size. **g.** There are no constraints.	This mesh approximates the mesh created in Tutorial A. Manhattan meshing will not work if variation to the shape (curved, tapered, or angled channels) results in a non-orthogonal structure.



Step 15: Create mesh	
User	**Explanation**
a. Click **Create Mesh**. This process may take several minutes. **b.** When the AutoMesher is finished, the Visualizer will open. Select the *Front View* and middle-click on the object to display the mesh. **c.** The default name of the part is *invert_1*. Change this to *Fluid*.	This mesh will not be visually identical to that created in the previous tutorial, but will provide the same simulation results.



Step 16: Change part status	
User	**Explanation**
a. In the panel on the left, observe that the Material is *UNDEFINED* and the Status is *movable*. **b.** Use the drop-down menu to change the status to *fluid*. **c.** Click **Update** to update the file.	Since the water in this simulation is fluid, the status must be changed. The change may be made either at this point, or in Step 18.

4.3.6: Changing Patch Names

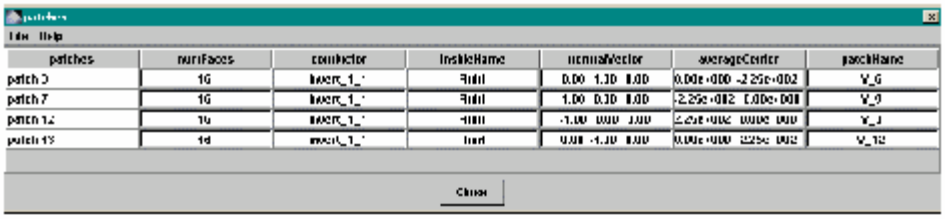
Step 17: Rename channel end patches	
User	**Explanation**
a. Click *Patches*. **b.** Middle-click on the object. The default name *patch_4* will appear in the *Name* field. Select **Hide Selected Patch**. **c.** Select the *Isometric view*. **d.** From the menu bar, select *Edit* > *Edit model*, change the Z scale to 50, and click **Update**. **e.** **Close** the *Edit Model* dialog box. **f.** Rename the channel end patches using the same patch names used previously. Review Step 7 of the previous tutorial if necessary. **g.** Select *File* > *save* to save the changes, and *File* > *Quit* to close the Visualizer.	Patch names are changed to correspond to positions on a clock for ease of reference.

4.3.7: Solver and Tool Setup

Step 18: Check the Model Type	
User	**Explanation**
a. Select the *Analysis* tab of the Function Manager. **b.** Select the *Microfluidics Solvers* Category and the *SwitchSim* Type. **c.** Select *switchcross-invert.mbif* from the drop-down menu if it does not appear by default in the Input field. Select the *View MBIF* icon at the right end of this field. **d.** Under Model Info, select *names*. **e.** Verify that the Model Type is *fluid*. **f.** Click **OK**.	The simulation will not run if the Model Type is *movable*.

Step 19: Change volumeMaterials	
User	**Explanation**
a. Under Model Info, select *volumeMaterials*. **b.** Under *Material*, click on **UNDEFINED** to open a dialog box **c.** In the *Material* field, click the arrow to the right to open a drop-down menu. **d.** Select **Water**. **e.** Click **Read From Database** to populate the table with material characteristics for water. **f.** Click **Close**. **g.** Click **OK** to close the *volumeMaterials* dialog box.	The fluid that fills the channel and transports the species must be defined. In this step, the properties of water are assigned to the channel volume.

Step 20 : Verify patch names	
User	**a.** Select *patches* and ensure the four channel end patches have been named correctly. **b.** Click **Close**. **c.** Click **Done** to close the *Model Info* panel.



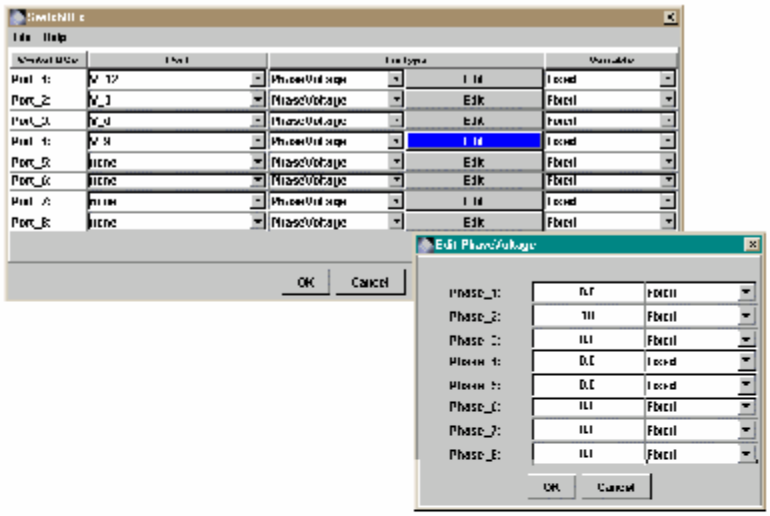
4.3.8: Solver and Tool Setup

From this point, the procedure is the same as that in Tutorial A except for two values in the SwitchSim boundary conditions.

Step 21 : Use Boundary Conditions from previous tutorial	
User	**a.** Select **Solver Setup...** to open the *Tool* window. **b.** Refer to steps 10 through 14 (page 57) of Tutorial A for Boundary conditions. **c.** When the *Phase* parameters have been set, click **OK** to close the *Phases* dialog box. **d.** Proceed with Step 22 to set the Switch boundary conditions.

4.3.9: Setting SwitchSim Boundary Conditions

Step 22: Set Switch Boundary Conditions	
User	**Explanation**
a. Select **SwitchBCs** from the SwitchSim BCs control panel. **b.** Edit the Phase voltages according to these settings: Port 1 V_12 Phase 1: 0 Phase 2: 0 Port 2 V_3 Phase 1: 18 Phase 2: 18 Port 3 V_6 Phase 1: 0 Phase 2: 18 Port 4 V_9 Phase 1: 0 Phase 2: 18 Click **OK** to close each *Edit Phase Voltage* dialog box after entering the correct values.	In Tutorial A, the Phase 1 voltages for Ports 1 and 3 were set at 9. These values are reduced to 0 volts in this simulation to induce pinch.



Step 23: Begin Simulation	
User	**Explanation**
a. Click **OK** to close the SwitchBCs dialog box. **b.** At the bottom of the SwitchSim BCs control panel, click **Simulate**. **c.** Click **OK** to save settings when prompted.	It is a good idea to save settings so that in the event of a system problem, the boundary conditions and other factors will not have to be re-entered.

4.3.10: Simulation Results

Step 24: View Graph	
User	**Explanation**
Open spIntegral Graph and compare results with Tutorial A	The graphs are presented in Figure 4-6 and Figure 4-7.

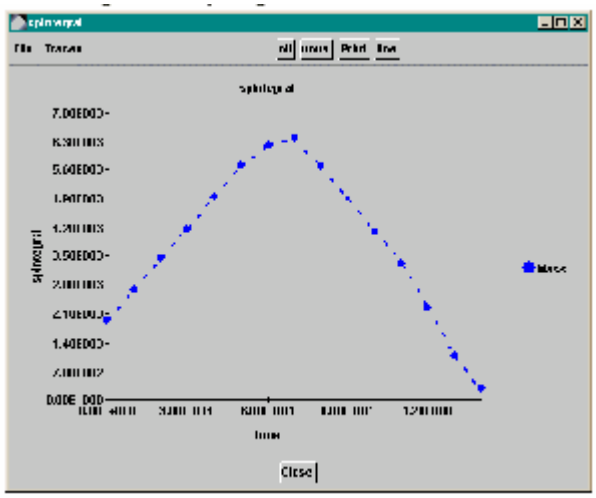


Figure 4-6 spIntegral Results from Tutorial A

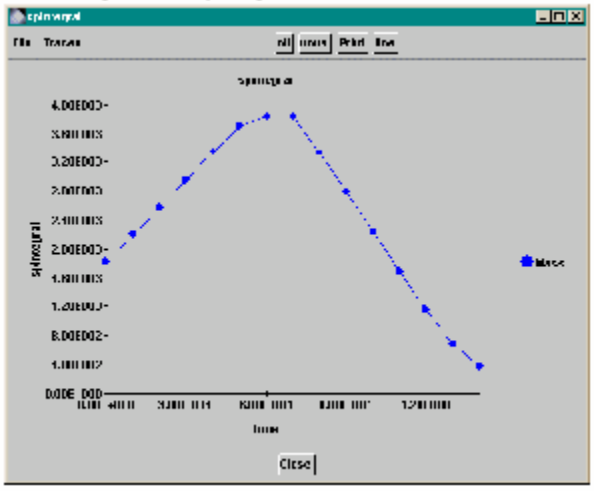
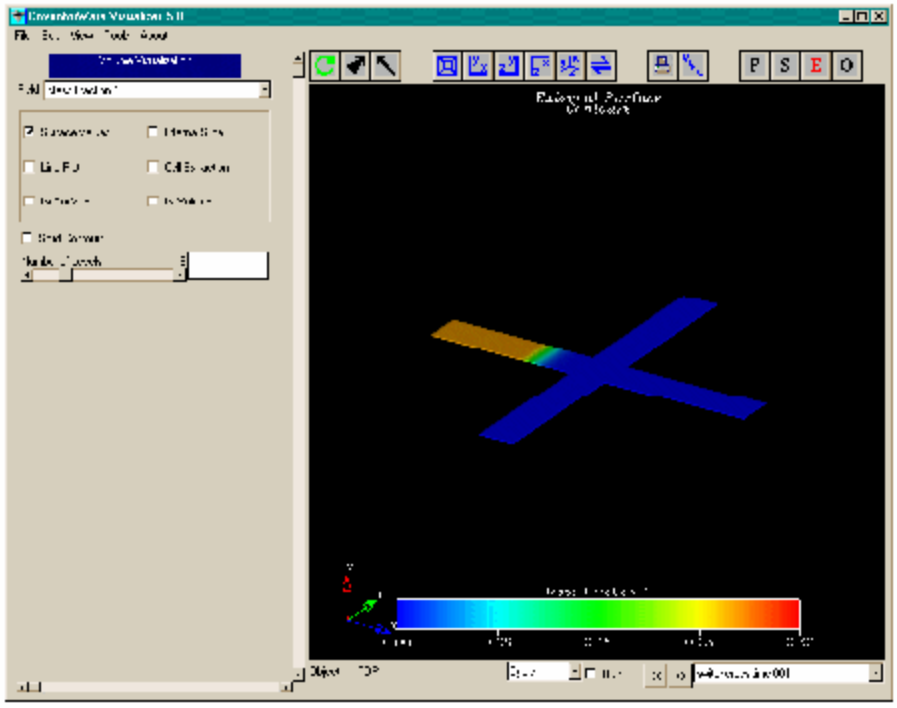


Figure 4-7 spIntegral Results from Tutorial B

Step 25: View the Simulation Results	
User	**Explanation**
a. Start the Visualizer **b.** Select **Visualize list**. **c.** Select *isometric view* and *normalize*. **d.** Click on the **E** icon for volume visualization **e.** Select *Edit>Edit MBIF* **f.** Click on *Active Fields* **g.** Uncheck the *Mises* and *Displacement* fields **h.** Check the *Mass Fraction 1* field. **i.** Click on **Update** and then **Close** the window.	At this point, there is no observable difference between the visible results and those obtained in Tutorial A.



Step 26 : Compare and contrast results	
User	Step through the list using the >> icon until switchcross time 006 is displayed. Compare this view with the view following Step 19 of Tutorial A. Observe the effect of pinch on the model.

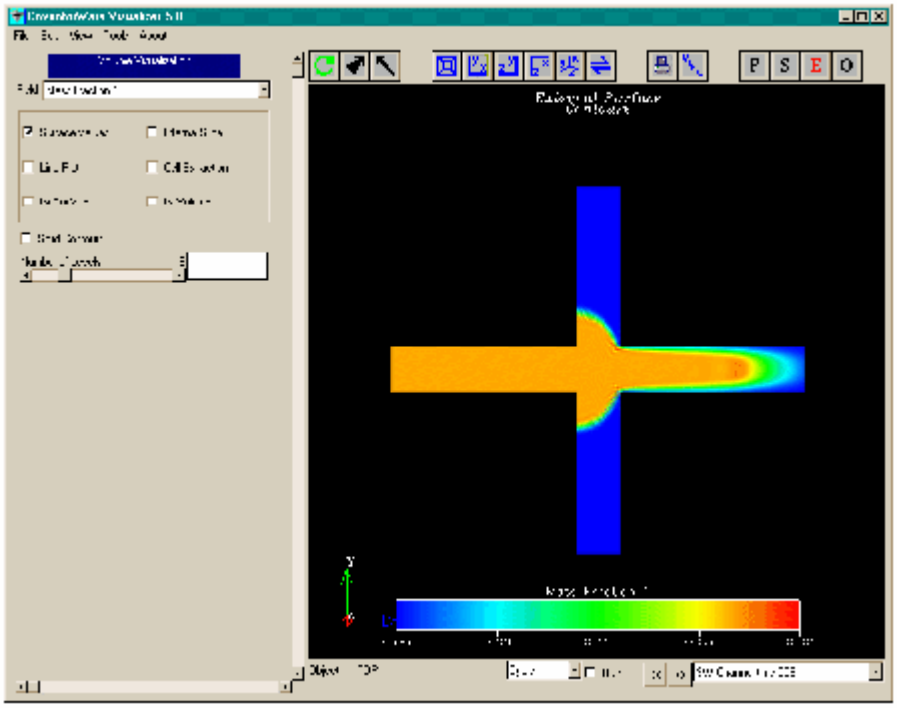


Figure 4-8 Species Without Pinch

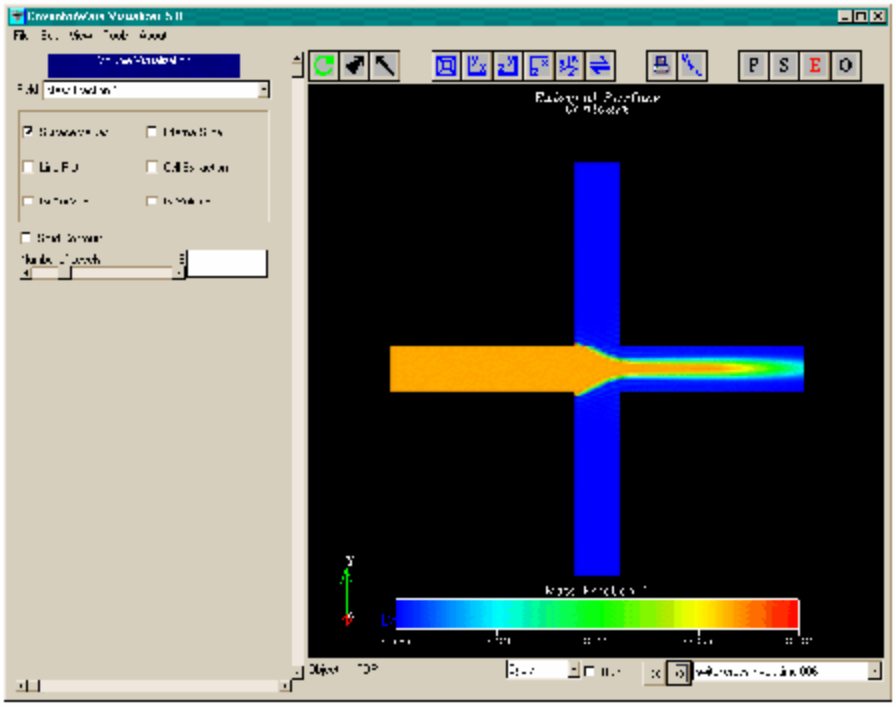


Figure 4-9 Species With Pinch

Step 27: Further Analysis	
User	**Explanation**
The post-simulation analysis steps of Tutorial A can be duplicated here if desired.	This simulation can be repeated with variations in voltage, time frame, density or switch configuration.

4.4: Reference

This section explains the SwitchSim windows and the setting options available in each one. The window map in Figure 4-10 is an overview of the SwitchSim solver flow.

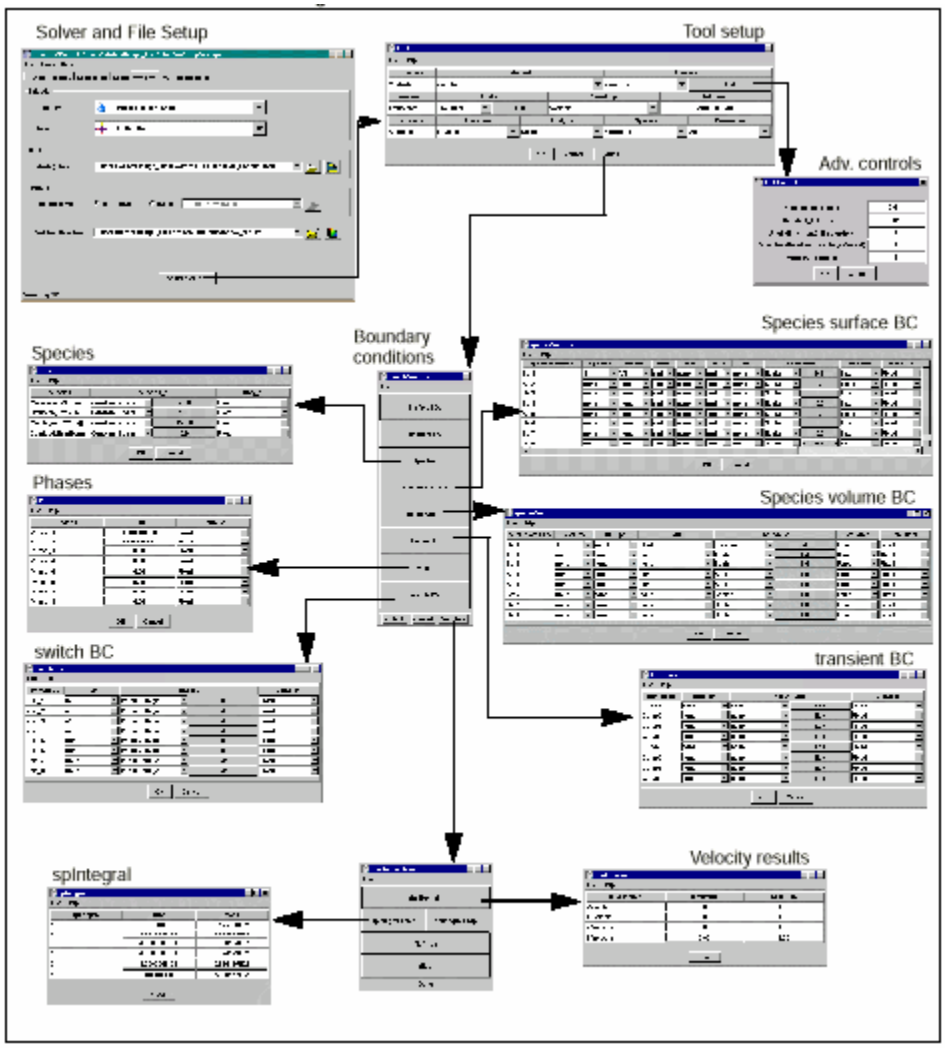
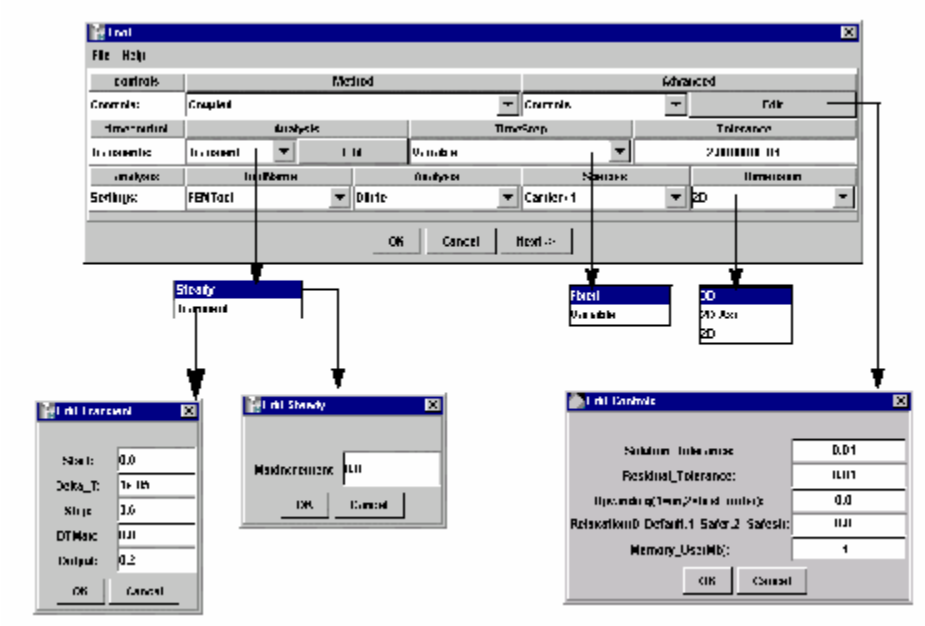


Figure 4-10 SwitchSim solver flow

4.4.1: Tool Window

When the user selects the SwitchSim solver the Tool window allows the user to set the parameters for running the fluidic solver.



- **Controls/Method**

The Navier-Stokes equations used in the microfluidics solvers are non-linear and require an iterative approach to solving problems. The solvers adjust a variety of variables as part of the solution method, allowing them to solve both straightforward problems with single solutions, as well as more complex problems with multiple local minimum or maximum values. This setting is only active for the FEM tool.

  - **Coupled**: The coupled solver is the default choice for the microfluidics solvers. This iterative solver is recommended for most problems, and can handle steady state and transient flows.
  - **Segregated**: The segregated solver solves each degree of freedom in the problem separately and consecutively. Thus, the three momentum equations for flow in the X, Y, and Z directions and the pressure and energy equations are each solved separately. This approach uses less system memory at the expense of a longer solution time. It is recommended for problems containing more than 1000 parabolic bricks.

- **Controls/Advanced Controls**

Several different tolerances may be set depending on the non-linearity of the flow problem.

  - **Solution Tolerance**: Convergence value setting. The default value of 0.0001 may be reduced if the solution is not fully converged.
  - **Residual Tolerance**: Applies only to the FEM tool. Similar to the Solution Tolerance; controls the Flux of a particular quantity.
  - **Upwinding**: A numerical solution stabilization technique that prevents solver instability. Occasionally, the solver will be unable to complete its calculations due to mesh anomalies. If this occurs, change this value to 1 (second-order stabilization) or 2 (first-order stabilization). FEMTool only.

- **Relaxation**: Specifies relaxation factors for the degrees of freedom in the system. The value of 0 is the default relaxation setting and is recommended for most solutions. The value of 1 is a more conservative setting, recommended for more difficult solutions such as a high Reynolds number or a high Peclet number. The value of 2 is the most conservative and is recommended for solutions that diverge when using the first two options. Optimal values are problem-dependent, and can be derived only by trial and error.
- **Memory Use**: The default setting is -1, which allows the software to allocate memory as required. For large 3-D problems, or to avoid unnecessary swapping, the user should set this value if the job is larger than the RAM memory. A suggested range is 2/3 to 4/5 of actual RAM. This setting applies only to the FEM tool. The FVM tool uses dynamic memory allocation; the solver allocates as much memory as it needs.

- **Transients/Analysis**

  - **Steady:** Performs a steady state or time-independent analysis. The solver will attempt to converge to an answer within the number of steps given in the Edit window MaxIncrement setting. The default value is 30, but the segregated solver may require that this value be increased.
  - **Transient:** This setting sets up the transient simulation. Five time steps are set: Start: Time to start simulation.
    Delta_T: Time interval for simulation. It should be set to a very small number, about 1e-6 times the Stop value for variable time steps. When using FVMTool or FEMTool/fixed timestep, Delta-T should be set using a Courant number. The Courant number is

$$C = \frac{V\Delta t}{\Delta x}$$

    where V is a characteristic velocity, delta X is the grid size, and delta T is the timestep. The Courant number should be less than 0.1 for accurate solutions. When using the Variable timestep, set Delta_T to a small value
    Stop: Time to stop simulation.
    DTMax: Applies only to the FEM tool. When TimeStep is set to Variable, sets the maximum range for the time step. If set to 0, it is ignored. It should be set to 0, except for complex problems, where it should be set to 1/100 of the total simulation time (0.01 * (Stop - Start)).
    Output: Specify time increments at which the mbif files are written. For example, a setting of 0.2 writes an mbif file every 0.2 seconds for the duration of the simulation.

- **Transients/TimeStep**

  This controls the time step of the overall transient analysis. The FVMTool always uses a fixed timestep.

  - Variable: This time stepping control default value is the optimal setting. The solver determines the time step value at any given point in the solution. With a variable setting, the solver can use small time steps at the beginning of the problem, and larger steps near the end when the solution is nearly complete.
  - Fixed: This time step is used for special problems. An example is when the solver would increase the timestep in the variable mode with steps that are larger than the time in which the effects that are studied occur. In highly viscous flows the actual start-up effects of the flow might be skipped. The Fixed time step also needs to be set if the Response option is used in the Transient Boundary Conditions. With the Response option the steady state situation is calculated first and switched off. Fixed timesteps are very efficient when using the coupled solver.

- **Transients/Tolerance**
  Tolerance of a physical time step in the transient analysis. Examining the mass conservation plot at the end of a transient simulation may check the accuracy of the solution. Depending on the mass conservation plot results, the tolerance value may be increased or decreased from the default setting of 0.001.

- **Analysis Settings/Tool name**

  - **FEMTool**: The FEMTool uses the Fidap solver. Fidap uses parabolic finite elements, and is more accurate for coarse meshes.
  - **FVMTool**: Uses the Fluent solver, which is capable of handling large models (hundreds of thousands of ele-ments), therefore allowing significant decrease in computation time and memory. The FVM tool gives more robust convergence for high Reynolds numbers or more complex flows. It also allows designers to use non-conformal meshing at fluid-fluid interfaces. Users can mesh different parts of the model with different tools, and then merge them into one model without worrying about nodes being coincident on the interfaces between separate meshes. This tool only supports linear bricks and linear tets. Three-dimensional meshes must be composed of linear bricks or linear tets. Two-dimensional meshes must be composed of linear bricks. Slip boundary conditions, volumetric velocity, and volumetric temperature boundary conditions are not supported with this tool.

    Use this tool for non-dilute problems, where the electrical conductivity is a function of the species concentration, or for coupled thermal electrokinetic problems where the electrical conductivity is a function of the temperature.

  - **Analysis Settings/Analysis**

    Sets the type of analysis to be performed. Dilute is the only choice.

  - **Analysis Settings/Species**

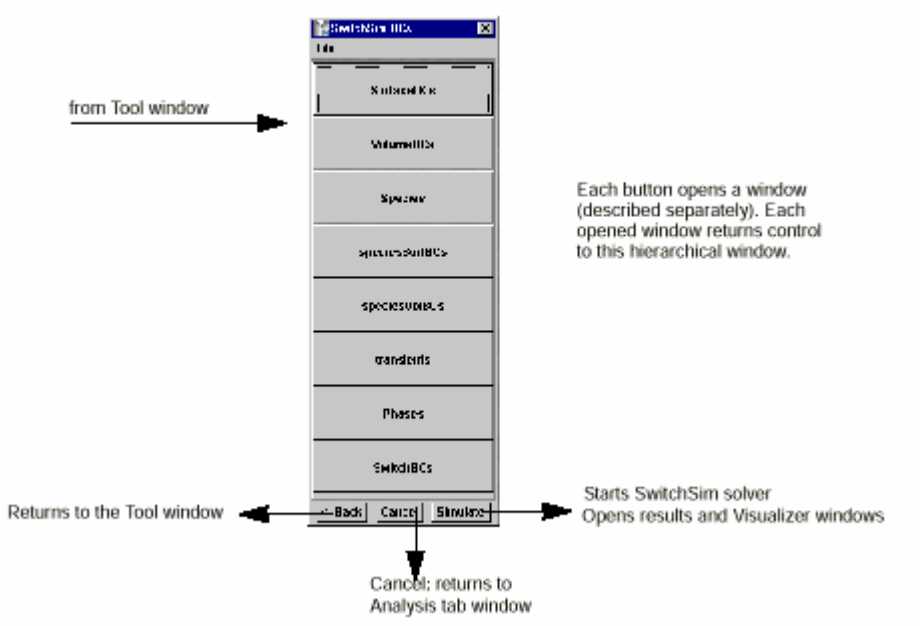
    Specifies the number of components present in the flow, including the carrier fluid. Choices are Carrier, Carrier+1, and Carrier+2.

  - **Analysis Settings/Dimension**
    - 3D: Tells the solver to run a three dimensional solution with dimensions X,Y, and Z.
    - 2D-Axi: Allows the user to run a two dimensional axi-symmetric solution. The model has to be generated in the XY-plane and should be 1 element thick in the Z direction. The X-axis is the axis of symmetry and the Y-axis is the radial coordinate.
    - 2D: Allows the user to run a two dimensional solution. The model has to be generated in the XY-plane and should be 1 element thick in the Z direction. No boundary conditions may be applied to surfaces, which lie in this X-Y plane.
  - **OK**
    Applies changes to the window, but does not continue with SwitchSim. Control returns to the Analysis tab window.

  - **Next**
    Applies the changes made in the Tool window; opens the SwitchSim boundary conditions window.

4.4.2: SwitchSim Boundary Conditions Window

The SwitchSim BCs boundary conditions window allows the user to choose windows to specify load conditions for the SwitchSim fluidic solver.



SurfaceBCs

Opens window (see page 94) to set surface boundary conditions, such as velocity and pressure.

VolumeBCs

Opens window (see page 97) to set boundary conditions that affect an entire volume, such as temperature conditions.

Species

Opens a Species window. Note that this button does not appear if the Tool window is set for a Species=1 value.

SpeciesSurfBCs

Opens window (see page 102) to set surface boundary conditions for species present in the carrier fluid.

SpeciesVolBCs

Opens window (see page 104) to set volume boundary conditions for species present in the carrier fluid.

Transients

Opens window (see page 106) to set conditions for transient calculations.

Phases

Opens window (see page 108) to set times when switching events occur.

SwitchBCs

Opens window (see page 109) to set switching voltages at the phase times specified in the phases window.

Simulate

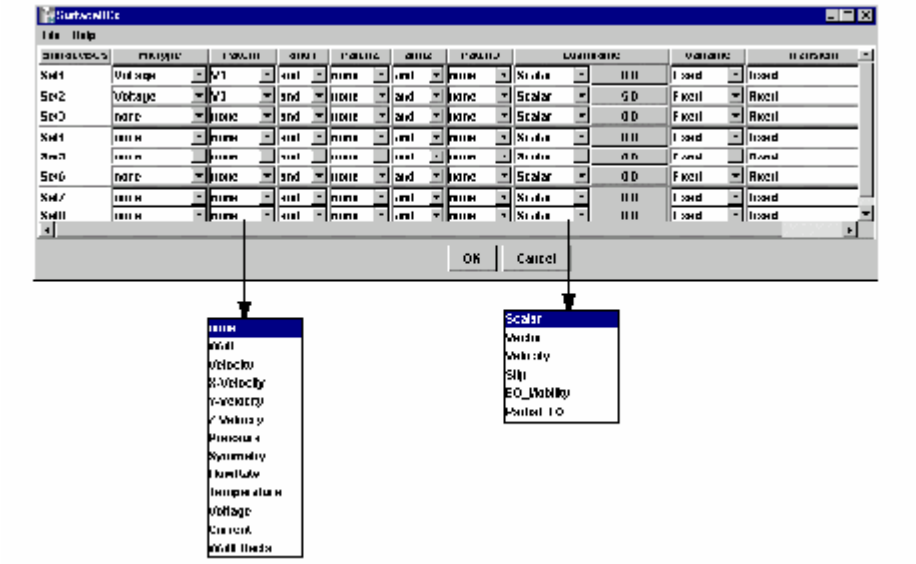
Launches SwitchSim solver.

Cancel

Does not proceed with SwitchSim solver; returns focus to Function Manager window.

Surface Boundary Conditions Window

The SurfaceBCs window sets patch surface boundary conditions. Fix types and load conditions for these surfaces can be specified in eight Sets within this window. When setting up conditions, the LoadValue button needs to correspond to the appropriate boundary condition. Not all combinations of boundary conditions and LoadValue can be used.



SurfaceBCs

This display-only column allows the user to define up to eight boundary condition sets for the model.

Fix Type

Enables pull-down menu with many load type choices:

- **Wall:** This represents a “no slip” (zero velocity) boundary condition at the selected patches. No LoadValue is applied.
- **Velocity**: Possible LoadValues are Velocity and Vector.
- **X-Velocity**: This option specifies a uniform velocity in the X-direction. The option is very useful when applying symmetric boundary conditions for which the velocity perpendicular to the axis of symmetry is 0. A Scalar LoadValue is used.

- **Y-Velocity**: This option specifies a uniform velocity in the Y-direction. The option is very useful when applying symmetric boundary conditions for which the velocity perpendicular to the axis of symmetry is 0. A Scalar LoadValue is used.

- **Z-Velocity:** This option specifies a uniform velocity in the Z-direction. The option is very useful when applying symmetric boundary conditions for which the velocity perpendicular to the axis of symmetry is 0. A Scalar LoadValue is used.

- **Pressure**: A constant pressure on the selected patch is specified. A Scalar LoadValue is used.

- **Symmetry**: The selected patch is a plane of symmetry. It is important that the entire problem, not just the geometry, is symmetric. No LoadValue is applied.

- **FlowRate**: The flow rate follows the sign convention of all boundary conditions. A positive flow rate is along the normal of the selected patch. In Coventor software the normal always points to the volume, so the FlowRate is into the patch when a positive value is specified. A Scalar LoadValue is used.

- **Temperature**: Applies a constant temperature on the selected patch. A Scalar LoadValue is used.

- **Voltage**: This boundary condition applies a constant potential on the specified patch. Note that a potential difference must be specified; therefore, two Voltage BC specifications are required. A Scalar LoadValue is used.

- **Current**: This boundary condition applies a current through the specified patch. A Scalar LoadValue is used.

- **Wall Effects**: This boundary condition allows the specification of electroosmotic effects in the flow. EO_Mobility LoadValues can be used. Slip wall effects also can be taken into account with the Slip Load-Value.

Patch1,2,3

Choose any of the patch names previously set up.

Load Value:

Choose from several load types. Each type uses a different edit window; the entire set of edit windows is shown as part of the LoadValue explanation.

- **Scalar**: one-dimensional quantity, such as pressure load or temperature.

- **Vector**: Used with the Velocity FixType. This defines a uniform velocity profile in the direction of the vector specified on the selected patch.

- **Velocity**: Used with the Velocity FixType. This is a quadratic, linear or constant polynomial in all three directions for the velocity on the selected patch. For each velocity U_x, U_y, and U_z a separate polynomial can be given. For example, Pouiselle Flow in a pipe yields the following profile:

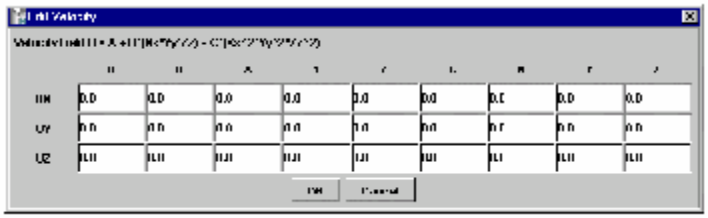
$$U = C\left[1 - \left(\frac{Y}{Y_0}\right)^2\right]$$

where C is a constant and Y_0 is the pipe radius.

For this example, the Edit Velocity window below requires that only the first U_x line needs to be filled in. The following column values are required for this window:

Column$A$ = C, Column$C$ = -C, Column$Y_y{}^2$ = 1. All remaining columns are zero.

The example shown is filled out for the constant C = 5.



- **Slip**: The Mean Free Path and the MAC (Momentum Accommodation Coefficient) are used in the slip equation to study wall effects in microchannels. It is used exclusively with the Wall Effects FixType. The slip velocity at the wall can be expressed as follows:

$$SlipVelocity = \sigma K \left(\frac{\partial U}{\partial n}\right)_{wall}$$

where U is the velocity, n is the direction normal to the velocity, σ is the streamwise momentum accommodation, expressed as follows:

$$\sigma = \frac{2 - \sigma_m}{\sigma_m}$$

where σ_m is the momentum accommodation coefficient (MAC). Usually, $\sigma_m = 1$ but it can vary within the range $0 < \sigma_m < 1$.

K is the Knudsen number, which can be expressed as:

$$K_n = \frac{MeanFreePath}{CharacteristicLength}$$

If this value is smaller than 0.01 the slip effect is neglected.

- **EO_Mobility**: This setting enables the representation of the electroosmotic effects on the walls through a mobility that defines the velocity achieved by the charged carrier at the edge of the double layer in the electric field. Note that this implies a relaxation of the no-slip wall boundary condition, since the near- wall region is no longer solved. The EO_Mobility is a positive number for a negatively charged wall. (In other words, a positive value will result in flow towards the negative electrode.)

- **Partial_EO**: This setting measures the EO mobility when the surface properties change across the length of a channel. To use this LoadValue with a specific patch, define a volume where the surface changes occur with the first six entries, and enter the new EO mobility for this region with the last entry.

Variable

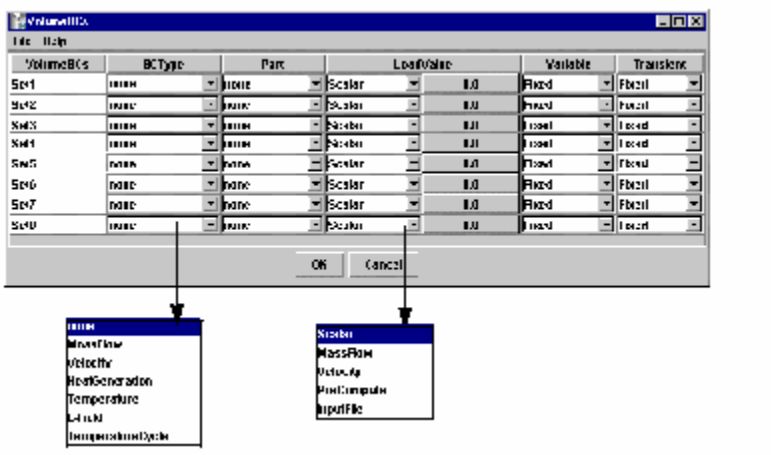
Setting for Simulation Manager. A Fixed setting (the default) uses constant Load Values, which are not changed during a Simulation Manager run. When a Load Value is to be a variable modified by a Simulation Manager trajectory, one of eight SW_BC variables can be used, corresponding to the lines in the SwitchSimBC Simulation Manager setup window.

Transient

Setting for transients surface boundary condition. A Fixed setting (the default) does not apply transients. When a Set is to be modified by a transient event, one of two Transient variables are available for assignment. The variable is defined in the transients window (see page 106). With this technique a periodic pressure or input flow can be generated. By setting the Transient variable the input on that node set is coupled to the waves or function defined in the transients window.

Volume Boundary Conditions Window

The VolumeBCs window sets volume boundary conditions. Types and load conditions for these volumes can be specified in Sets within this window.



VolumeBCs

This display-only column allows the user to define up to eight boundary condition sets for the model

BCType

Enables pull-down menu with several choices:

- **none**: Does not apply a boundary condition to the volume.
- **Mass Flow**: Specifies a mass flow in three directions—Mx, My, Mz. The Mass Flow LoadValue is used.
- **Velocity**: Applies a velocity to the selected part. A Vector, Velocity, or InputFile LoadValue is used.
- **Heat Generation**: Heat can be generated in a part. The part is usually a solid and not a fluid. A Scalar Load-Value is used.
- **Temperature**: Applies a fixed temperature to the selected part. A Scalar LoadValue is used.
- **E-Field**: The E-Field in the volume can be read from a pre-computed mbif file. Use the InputFile LoadValue and specify the directory path.
- **Temperature Cycle**: Applies a temperature cycle to the part.

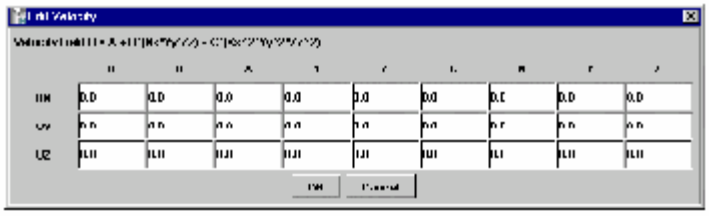
Part

Enables pull-down menu with a list of all the parts modeled and stored in the mbif file.

Load Value

Choose from several load types. Each type uses a different edit window, shown below with the LoadValue description.

- **Scalar**: Used to specify a one-dimensional value, such as Temperature or Heat Generation.
- **Mass Flow**: Used to specify a three-dimensional value for Mass Flow.
- **Velocity**: Used with the Velocity BCType. This is a quadratic, linear or constant polynomial in all three directions for the velocity on the selected part. For each velocity U_x, U_y, and U_z a separate polynomial can be given.



- **PreCompute**: Decouples the momentum and species equations. The velocity is pre-computed and an advection-diffusion analysis for the species follows. No LoadValue edit window is used.
- **Input File**: Specifies a result mbif file from another simulation as the source data input initial conditions. The default directory is the directory from which the software is launched.

Variable

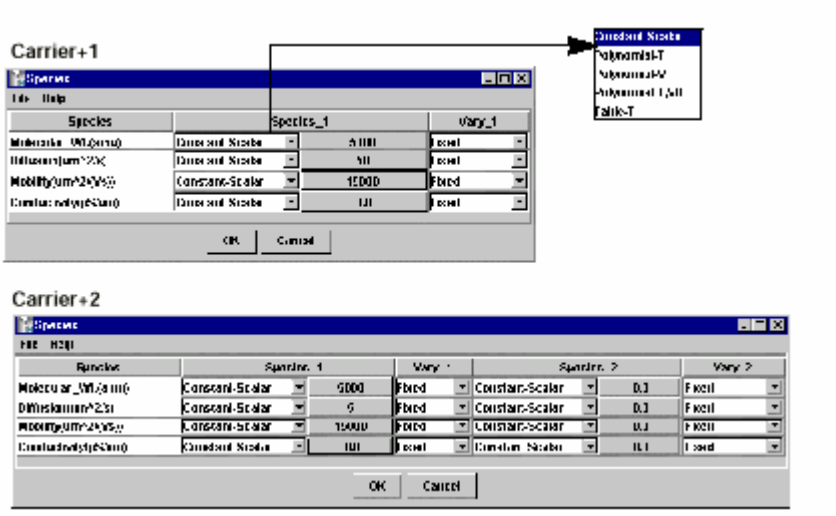
Setting for Simulation Manager. A Fixed setting (the default) uses constant Load Values, which are not changed during a Simulation Manager run. When a Load Value is to be a variable modified by a Simulation Manager trajectory, one of eight SW_BC variables can be used, corresponding to the lines in the SwitchSimBC Simulation Manager setup window.

Transient

Setting for transients surface boundary condition. A Fixed setting (the default) does not apply transients. When a Set is to be modified by a transient event, one of two Transient variables are available for assignment. The variable is defined in the transients window (see page 109).

Species Window

The Species window allows the user to specify the species characteristics used for the simulation. The species present are in infinitely dilute form, therefore material properties are not needed. The Tool window must have Species set to Carrier+1 or Carrier+2 to access this window. Carrier+1 results in a single-column Species window, and Carrier+2 results in a dual-column Species window.



species

This view-only window lists the species parameters that user can specify for simulation: Molecular Weight, Diffusion, Mobility, and Conductivity.

Species_2, Species_3

Designates the type of parameter to be specified. Choices include:

- **Constant-Scalar**: Constant with a single value over the entire field.
- **Polynomial-T**: Polynomial function of temperature. Six constant coefficients are allowed to enable the definition of up to a fifth order polynomial.
- Polynomial-V: Solves for non-linear electrophoresis. The user enters up to six polynomial coefficients.

  For non-linear electrophoresis problems where the electrophoretic mobility changes significantly, oscillations may be observed in the solution. These can be damped out by turning on Upwinding (from the Advanced button in the Tool window) and setting the value to 1. After running a simulation, the user should check the spIntegral results table carefully. It may be necessary to adjust the Tool window Timestep to Variable, and the Tolerance value downwards (in the range of 1.0e-03 to 1.0e-06) to improve mass conservation.

- **Polynomial-T,V0**: This setting is not currently supported in SwitchSim.
- **Table-T**: Tabular form for defining temperature-property pairs. Linear interpolation is used for intermediate values.

Edit window

Specifies the parameter value in this window. Window format dependent on the parameter type specified. The Edit window variants are shown on page 104.

Species Edit windows

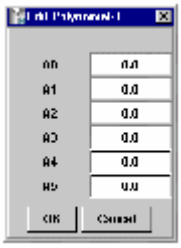
Each LoadValue type selected from the Species window uses its own format for entering parameters. The windows are described in more detail in this section.

Constant-Scalar

Constant with a single value over the entire field.

Polynomial-T

Polynomial function of temperature. Six constant coefficients are allowed to enable the definition of up to a fifth order polynomial.



Polynomial-V

Polynomial function of electric field strength. Used to calculate non-linear electrophoresis. The user enters up to six polynomial coefficients.

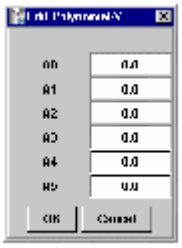
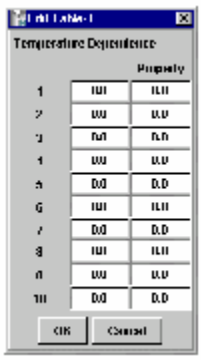
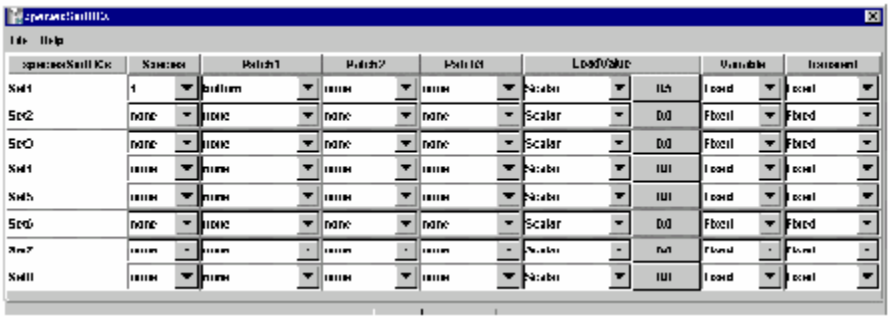


Table-T
Tabular form for defining temperature-property pairs. Linear interpolation is used for intermediate values.



Species Surface Boundary Conditions Window

The speciesSurfBCs window sets surface boundary conditions for the species. Fix types and load conditions for these surfaces can be specified in eight Sets within this window. When setting up conditions, the LoadValue button needs to correspond to the appropriate boundary condition. Not all combinations of boundary conditions and LoadValues are possible.



speciesSurfBCs

This display-only column allows the user to define up to eight boundary condition sets for the model.

Species

Can choose either Species 1 or Species 2 for the setting.

Patch1,2,3

Choose from any of the patch names previously set up.

Load Value

Choose from several load types. Each type uses a different edit window; the entire set of edit windows is shown
as part of the LoadValue explanation.

- **Scalar**: a fixed value on a patch.
- **Inj_Gaussian**: the injection of a finite width Gaussian stream of species through the patch. The Full-Width at Half Max (FWHM) value can be defined in seconds or in microns.

- **Inj_Plug**: the injection of a finite width square plug through the patch. The Length of the plug can be defined in seconds or in microns.

Variable

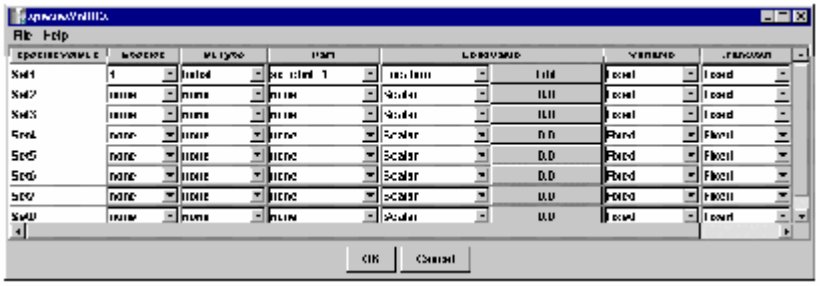
Setting for Simulation Manager. A Fixed setting (the default) uses constant Load Values, which are not changed during a Simulation Manager run. When a Load Value is to be a variable modified by a Simulation Manager trajectory, one of eight SW_BC variables can be used, corresponding to the lines in the SwitchSimBC Simulation Manager setup window.

Transient

Setting for transients surface boundary condition. A Fixed setting (the default) does not apply transients. When a Set is to be modified by a transient event, one of two Transient variables are available for assignment. The variable is defined in the transients window. With this technique a periodic pressure or input flow can be generated. By setting the Transient variable the input on that node set is coupled to the waves or function defined in the transients window.

Species Volume Boundary Conditions Window

The speciesVolBCs window sets volume boundary conditions for the species. Types and load conditions for these volumes can be specified in Part sets within this window.



speciesVolBCs

This display-only column allows the user to define up to eight boundary condition sets for the model.

Species

Can choose either Species 1 or Species 2 for the setting.

BCType

Enables pull-down menu with several choices:

- **none**: Does not apply a boundary condition to the volume.
- **Fixed**: Fixes the selected volume.
- **Initial**: This boundary condition is used only for transient flow analysis. A patch needs to be associated and selected in order to pose a numerically correct problem. The selected method enters Mass Fraction into the flow as desired. The transient problem needs a Dirichlet BC for the concentration, which is chosen to be 0 on the selected patch. Thus, the selected patch should be far enough upstream in order for the Mass Fraction not to reach the patch at any time.

Part

Enables pull-down menu with a list of all the parts modeled and stored in the mbif file.

Load Value

Choose from several load types. Each type uses a different edit window, shown below with the LoadValue description.

- **Scalar**: Used to specify a one-dimensional value, such as Temperature or Heat Generation.

- **Location:** Confines the concentration, given by the Mass Fraction, to the selected minimum and maximum values of X, Y, and Z. The software finds all nodes that are within these bounds and applies the Mass Fraction. If the minimum and maximum in any direction are left unchanged (i.e. zero), it means that “no filter” is applied in this direction. Using this LoadValue can lead to solver uncertain-ties, due to the sharp edges created by the Location setting. The Gaussian setting is preferred.

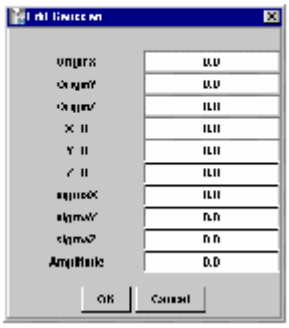
- **Gaussian**: Applies a Gaussian distribution according to the following formula:

$$A\exp\left[\left(\frac{x-x_0}{\sigma_x}\right)^2\right]\left[\left(\frac{y-y_0}{\sigma_y}\right)^2\right]\left[\left(\frac{z-z_0}{\sigma_z}\right)^2\right]$$

  where A is the amplitude, and σ is the change in a particular direction. Typically, only one dimension is given a non-zero σ value, which results in a plug of species given a Gaussian distribution in one axial direction. The Gaussian setting greatly reduces solver instability, and is the preferred LoadValue for most calculations.

  The x_0, y_0, and z_0 values in the Edit Gaussian windows define a flat peak on the Gaussian plot in the x, y, and z-directions, respectively, from

$$-x0 \le (x - x0) \ge x0$$



- **Input File**: Specifies a result mbif file from another simulation as the source data input boundary conditions. The default directory is the directory from which the software is launched.

Variable

Setting for Simulation Manager. A Fixed setting (the default) uses constant Load Values, which are not changed during a Simulation Manager run. When a Load Value is to be a variable modified by a Simulation Manager trajectory, one of eight SW_BC variables can be used, corresponding to the lines in the SwitchSimBC Simulation Manager setup window.

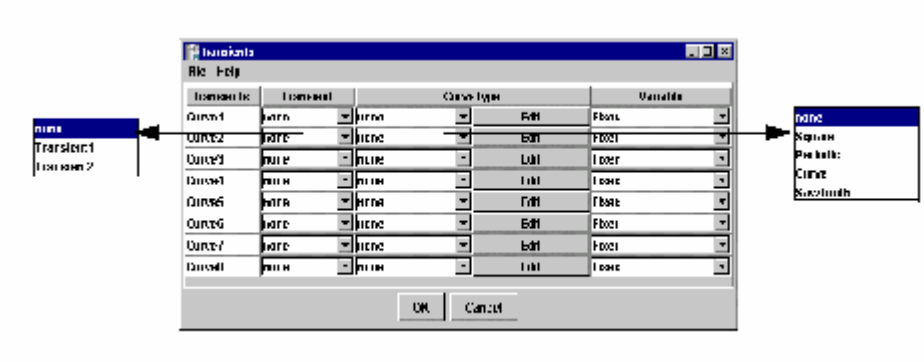
Transient

Setting for transients surface boundary condition. A Fixed setting (the default) does not apply transients. When a Set is to be modified by a transient event, one of two Transient variables are available for assignment. The variable is defined in the transients window.

Transients Boundary Conditions Window

The transients window enables the user to specify boundary conditions associated with transient calculations. Transient variables can be assigned in the SurfaceBCs or VolumeBCs window, and the type of transient response to use for the problem can be specified in this window. Two different transient types can be specified. For any transient analysis, the appropriate parameters should be set up in the SwitchSim Tool window.

> Transients are restricted to the following boundary condition settings: SurfaceBCs—Velocity, X,Y,Z Velocity, Pressure, FlowRate Temperature, Heat Flux, Concentration; VolumeBCs—Heat Generation.



transients

This display-only column allow the user to define up to eight boundary condition transient sets for the model.

Transient

This column allows assignment of one of two transient curve variables: Transient1 or Transient2. The equivalent TransientBC1 and TransientBC2 variables are assigned in either the SurfaceBCs or VolumeBCs window to a desired parameter for transient analysis.

Curve Type / Edit

The SwitchSim transient capability allows one of four different transient waveforms to be specified for the analysis. The specific waveform characteristics are specified in the Edit window accessed from the Edit button. These Edit windows are further described below.

- Square: Assigns a square wave as the transient curve. The square wave can be controlled by adjusting its period, split (duty cycle), or amplitude.
- Periodic: Assigns a periodic curve as the transient. The periodic curve can be controlled by adjusting its period, mean, or amplitude.
- Curve: Assigns a table of time step and property values in order to create a customized curve.
- Sawtooth: Produces a sawtooth waveform.

Variable

Setting for Simulation Manager. A Fixed setting (the default) uses constant Load Values, which are not changed during a Simulation Manager run. When a Load Value is to be a variable modified by a Simulation Manager trajectory, one of two FluidBC variables can be used, corresponding to the lines in the fluidBCs Simulation Manager setup window.

Transients BC Edit CurveType Windows

Each transient LoadValue type selected from the Edit CurveType window uses its own format for entering parameters. The windows are described in more detail in this section.

Square

The square wave can be controlled by adjusting its period, split (duty cycle), or amplitude. Period is the time between the start of two consecutive square waves. Split is a value between 0 and 1. If Split is 0.5, the square wave is at its maximum for half a period. If the Split is 0.3, then the square wave is at its maximum for 30% of the period. Amplitude is the maximum value of the square wave.

Periodic

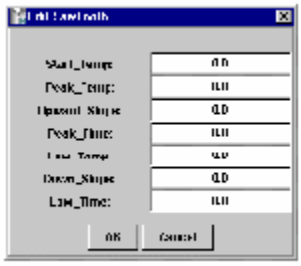
The periodic wave can be controlled by adjusting its period, mean, or amplitude: Period is the time between the start of two periodic waves. Mean moves the periodic curve vertically (up or down). Amplitude is the maximum value of the periodic wave.

Curve

The custom curve is described with a table of time step and property values. Users can enter up to 10 different sets of time and amplitude values to simulate almost any type of transient curve.

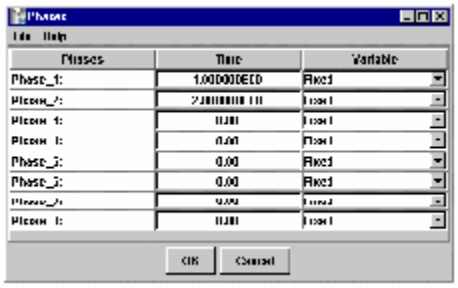
Sawtooth

The sawtooth is described with a combination of time and temperature values, along with a slope specification for the sawtooth angle.



SwitchSim BCs / phases boundary conditions window

The tables allow the user to set the switching time intervals for the simulation sequence. The voltages corresponding to each phase are set in the switching boundary conditions window.



Phases

This display-only column allows the user to define up to eight different phase times for switching to occur.

Time

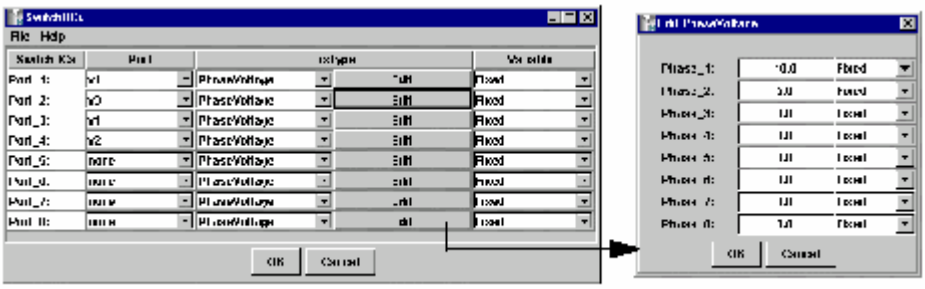
This column allows assignment of a phase time. Times specified are intervals; the cumulative event time is the sum of all specified phase times. The solver stops at the first phase duration time of 0.0. The total simulation time is equal to the sum of the phases.

Variable

Setting for Simulation Manager. A Fixed setting (the default) uses constant Load Values, which are not changed during a Simulation Manager run. When a Load Value is to be a variable modified by a Simulation Manager trajectory, one of eight SwSimBC variables can be used, corresponding to the lines in the SwitchSimBC Simulation Manager setup window.

SwitchBCs Boundary Conditions Window

The SwitchBCs window allows the user to set the voltage value for each port of the switch structure, with each Edit/array entry corresponding to the phase time set in the Phases boundary conditions window.



SwitchBCs

This display-only column allows the user to define up to eight port voltages for the switch structure.

FixType

This column allows assignment of either PhaseVoltage or PhaseCurrent as the phase type. The accompanying Edit button allows access to an Edit window. This additional window, shown above on the right, includes three columns:

- **array**: Read-only column with eight entries, corresponding to the eight possible phase time intervals in the phase table shown on page 108
- **Field**: Allows specification of a voltage or current value for that specific phase.
- **Sim**: Allows tagging the entry as Fixed or Variable for Simulation Manager use. Only the rows tagged as Variable in this window are affected by the SwSimBC variable assignment in the SwitchBCs window.

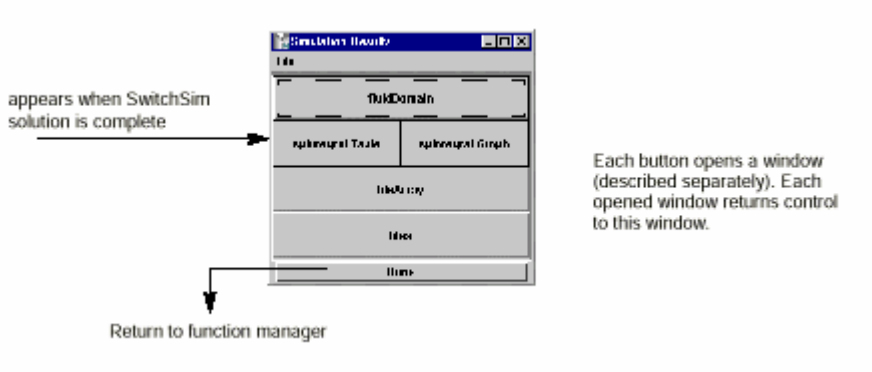
Variable

This setting is used for Simulation Manager. A Fixed setting (the default) uses constant Load Values, which are not changed during a Simulation Manager run. When a Load Value is to be a variable modified by a Simulation Manager trajectory, one of eight SwSimBC variables can be used, corresponding to the lines in the SwitchSimBC Simulation Manager setup window.

Only the rows tagged as Variable in the Edit window are affected by this variable assignment.

4.4.3: Simulation Results Window

The fluidic simulation results window allows the user to choose windows to view result tables and mbif file paths used during the computation.



fluidDomain

Opens window (see page 111) to display table of fluid results.

spIntegral Table

Opens window (see page 111) to display table of spIntegral results.

spIntegral Graph

Opens window (see page 111) to display graph of spIntegral results.

fileArray

Opens window (see page 112) to display directory paths of all saved mbif files.

files

Opens window (see page 112) to display directory path of solution results.

Done

Closes window and returns control to the function manager window.

File/Print

Enables printing of individual window results to a single file. The text format file can be used to interface to other programs such as Microsoft Excel. The file is located in the directory from which the software starts.

Fluid Solution Window

This fluidDomain window displays the results from the SwitchSim solver.

fluidDomain

Lists the type of velocity for the solver solution. Maximum velocity as well as the individual X,Y, and Z components are displayed.

Maximum

The maximum velocity calculated by the solver. The value shown is an absolute value.

Minimum

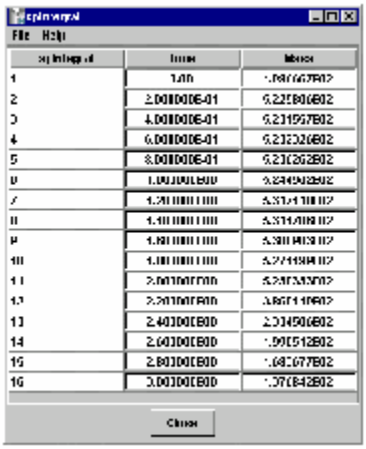
The minimum velocity calculated by the solver. The sign of the value is derived from the normal vector; a minimum value can represent maximum velocity. If the value in this column represents the maximum velocity for the model, the same value will appear in the Maximum column.

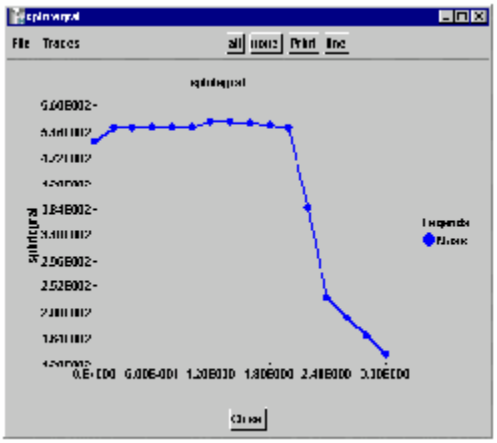
Close

Closes window and returns control to the hierarchical Simulation Results window.

SpIntegral Table and Graph Solution Windows

These windows display the numerical and graphical species mass results from the simulation. The transient time and output step settings for the table and graph are set in the SwitchSim Tool window.





spIntegral Time

This column and abscissa display the output step intervals set in the SwitchSim Tool window. In the above example, output mbif files are written every 0.2 seconds, and the mass results are displayed.

Mass

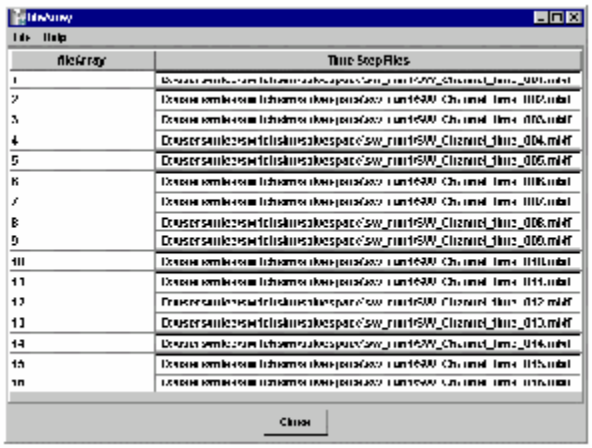
This column and ordinate display the species mass in the carrier fluid.

Close

Closes window.

Results / fileArray window

The FileArray window lists the directory paths for each output mbif file written during the simulation. The number of files is determined by the output time step length and total transient simulation run time, as set in the SwitchSim Tool window.



Result Files Window

This Files window displays the path to the result mbif file.

Section 5: ReactSim

5.1: Introduction

The ReactSim microfluidics module provides 3-D numerical modeling of multiple chemical reactions. These potentially competing reactions are modeled with full support for fluid flow coupling between species of varying densities, diffusion parameters, and electrokinetic variations. ReactSim supports chemical reactions in the volume of the fluid and/or on surfaces.

Applications include designing microchambers for chemical reactions and species transport, designing the containment of reactions in processing nodes, making detailed quantitative measurements of microchemical flows to calibrate and validate simulations, and building on-chip bio-assays for genetic diagnostics or environmental monitoring.

5.2: Tutorial

This simple tutorial deals with the study of gas-liquid catalytic reactions in flat plate microchamber reactor. In this reactor, gas and liquid reactants are brought into contact through a porous membrane. A catalyst deposited in the opposite wall enables the reaction between species. The tutorial shows how to design such a channel by having the user perform parametric studies of channel dimensions, the reaction rate constants, and the diffusion coefficients. The simple reaction chamber is shown in Figure 5-1. Inlet, outlet, and wall boundaries are used for species introduction and transport.

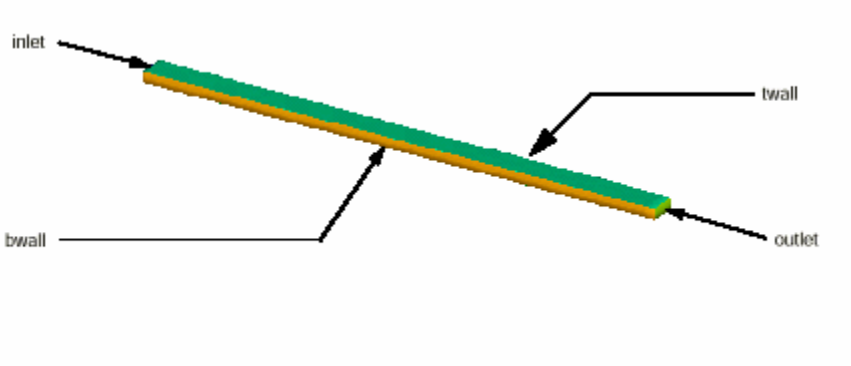


Figure 5-1 Initial chamber model with patches identified

5.2.1: Initialization

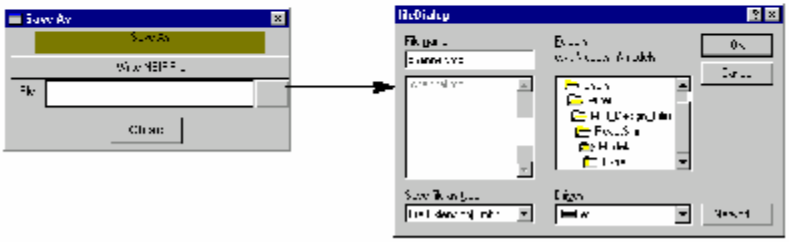
Step 1 Create a new project directory	
User	**Explanation**
a. Start Coventor software. **b.** In the Projects window that opens, select the *Import Tutorials* icon. **c.** In the window opens, select *ReactSim*. **d.** Click on **OK**. **e.** In the Projects dialog window, select the *ReactSim* project directory. **f.** Click on **Open**.	– When you select the *ReactSim* directory, the software copies this directory to your work directory. All the files needed for the tutorial are stored in this directory, and the software defaults to the appropriate directories when looking for a file. For details on file organization, refer to the File Organization section in the Reference Guide. – The software also creates a default settings file named *ReactSim.mps*.

5.2.2: View MBIF

In this section, you will need to rename two patches on the installed channel.mbif model so the proper boundary conditions may be applied.

Step 2: Set up file window	
User	**Explanation**
a. In the function manager window, click on the *Analysis* tab. **b.** Set your *Input Mesh* file path to the *channel.mbif* file in the *ReactSim/Devices* directory. **c.** Click on **View MBIF**.	– You need to access the Visualizer to rename patches for the simulation.

Step 3: View MBIF tasks	
User	**Explanation**
a. In the Visualizer Control panel menu window, click on **Start Visualizer**. **b.** Set the display for a normalized isometric view using  and	– The wall patches are renamed so they can be distinguished for boundary condition setup. – See Figure 5-2 for identification.
c. With the middle mouse button, click on the near side surface named *wall*. **d.** Change the name to *bwall*; click on **Update**. **e.** Hide the top wide patch. **f.** Middle click on the now-visible far side surface also named *wall*. **g.** Change the name to *twall*; click on **Update**.	
h. Click on *File* at the top of the Visualizer window. **i.** From the pull-down menu, click on *Save As*. **j.** In the SaveAs window that opens, click on the  button. **k.** In the fileDialog window that opens, navigate to your *ReactSim/Devices* directory. **l.** Name the new file *channelr.mbif*; click on **OK**. **m.** Back in the SaveAs window, click on **Write MBIF File**. **n.** In the Visualizer Control Panel window, click on **Stop Visualizer**. **o.** Click on **Done** in the Model_Info window.	– You have provided new names to the former *wall* patches, and saved the work in a new mbif file.



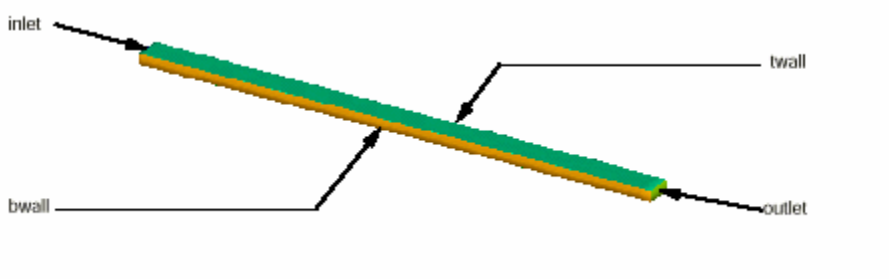
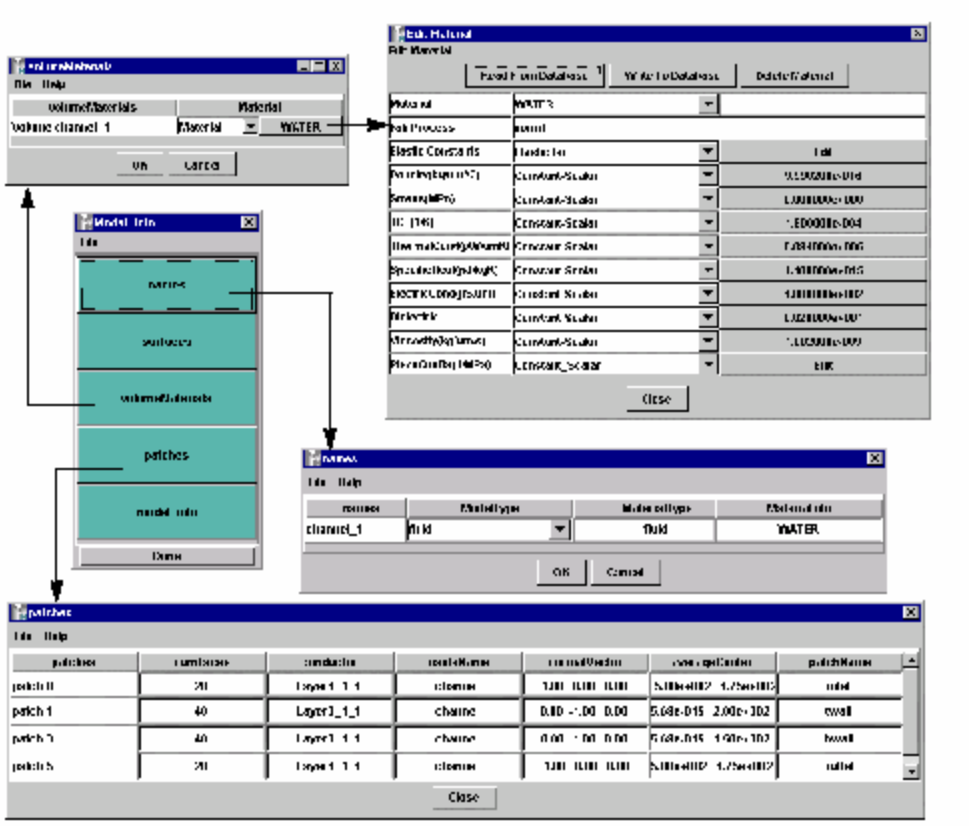


Figure 5-2 New patch Names for channelr.mbif File

Step 4: Set up and review ReactSim parameters	
User	**Explanation**
a. From the Analysis tab, change the *Input Mesh* file field to the *channelr.mbif* file you just created. **b.** Click on the **View MBIF** icon. **c.** From the Model_Info window, click on **names**, and review the window. **d.** Click on **OK**. **e.** Click on volumeMaterials. **f.** Click on *WATER* and verify the material properties for water shown in the Edit Material window. **g.** Click on **Close** in the Edit Material window and on **OK** in the volumeMaterials window. **h.** Click on **patches**. **i.** Review the listing against the diagram shown in Figure 5-2 **j.** Click on **Close**. **k.** Click on **Done** in the Model_Info window.	– These windows are unchanged from those in the initial MemCFD tutorial, with the exception of the new patch names.

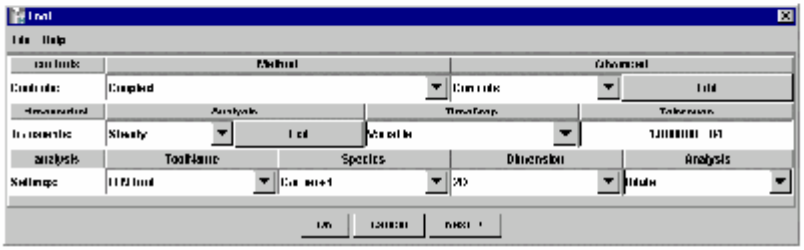


5.2.3: ReactSim

Use ReactSim, to set up the parameters for channel analysis.

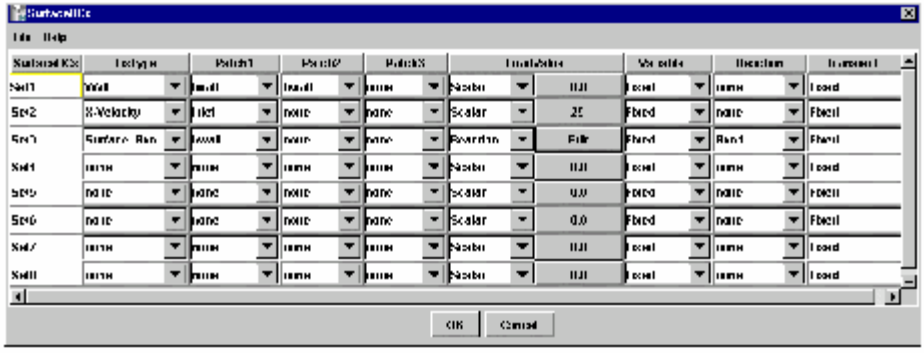
Step 5: Set up ReactSim Model window	
User	**Explanation**
a. In the Analysis window, select *Microfluidics Solvers* from the *Category* pull-down menu. **b.** Select *ReactSim* from the *Type* pull-down menu. **c.** Set the *Execution Mode* to *Interactive*. **d.** Create a solutions directory in your *ReactSim/Solutions* path to store the mechanical results. Name it *rs_run1*. **e.** Click on **Solver Setup**.	– This tutorial uses the mhif file you created in the first MemCFD tutorial.

Step 6: Set up ReactSim Tool window	
User	**Explanation**
a. Set the ReactSim Tool window for *Steady* state with a *Variable* TimeStep. **b.** Set for a *2D* analysis using a *Carrier+3* species setting. **c.** Set the remaining fields as shown. **d.** Click on **Next**.	– The window is set for transport of a carrier fluid, 2 species for reaction, and a third species as the reaction product.

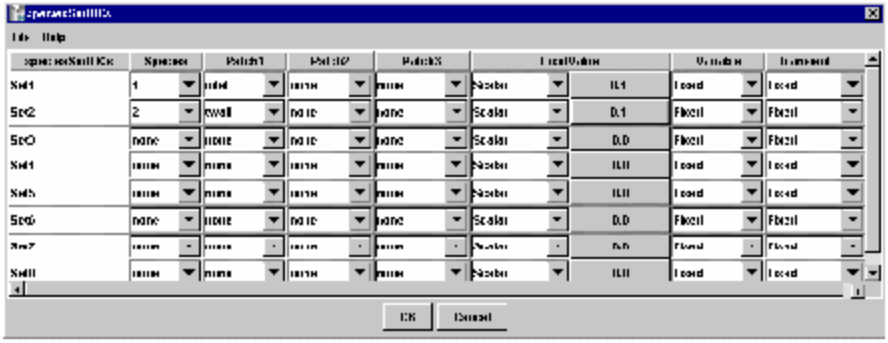


Step 7: Set up and review ReactSim Species parameters	
User	**Explanation**
a. From the ReactSim BCs window, click on **Species**. **b.** Set the species conditions as shown in the window. **c.** Click on **OK**	– You are setting the parameters for the 3 species declared in the Tool window. – The species product requires only a Diffusion setting.

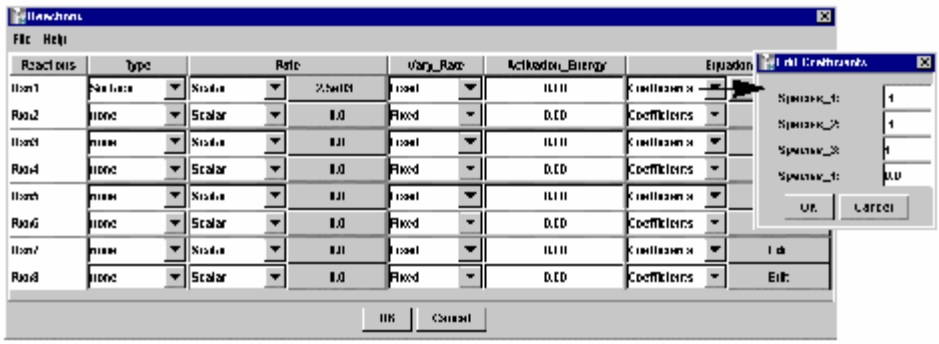
Step 8: Set up and review ReactSim surface boundary conditions	
User	**Explanation**
a. From the ReactSim BCs window, click on **SurfaceBCs**. **b.** Set a *Wall* FixType for the patches *twall, bwall* (use the *or* designation). **c.** Set a *X-Velocity* FixType for the patch *inlet*; set a scalar value of *25*. **d.** Set a *Surface_Rxn* FixType for the patch *bwall*; also set a *Reaction* LoadValue and a *Rxn1* Reaction type variable. **e.** Click on **OK** in the SurfaceBCs window.	– Species 2 enters through the *twall* boundary, Species 1 enters through the inlet with the specified velocity, and the reaction is set to occur at the bottom *bwall*. The Reactions window defines the *Rxn1* variable.



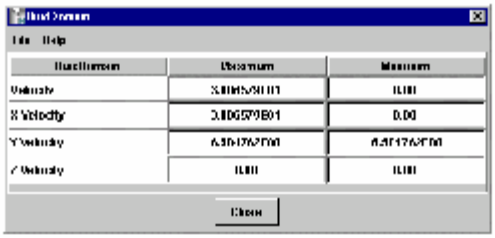
Step 9: Set up and review ReactSim species surface boundary conditions	
User	**Explanation**
a. Click on **speciesSurfBCs**. **b.** Set Species *1* to the *inlet* patch and a LoadValue of *0.1*. **c.** Set Species *2* to the *nwall* patch and a LoadValue of *0.1*. **d.** Click on **OK** in the speciesSurfBCs window.	- Concentration values are assigned.



Step 10: Set up and review ReactSim reaction parameters	
User	**Explanation**
a. Click on **Reactions**. **b.** Set a *Surface* reaction with a reaction rate of *2.5e03*. **c.** Set the Species coefficients as shown. **d.** Click on **OK** in the speciesSurfBCs window. **e.** Check the VolumeBCs, speciesVolBCs, and transients windows to be sure they are inactive. **f.** In the hierarchical window, click on **Simulate**.	- You are defining the parameters for the reaction variable *Rxn1* that you previously assigned for the *Surface_Rxn* boundary condition. - The Coefficients (A,B,C,D) are used in the equation nA + mB = pC + qD. The reactants must be negative numbers, while the product must be positive.



Step 11: View the ReactSim table results	
User	**Explanation**
a. In the Simulation Results window click on **fluidDomain** to view the simulation results. b. Click on **Close**.	– The window lists the maximum and minimum velocities in the X,Y, and Z direction for pressure driven flows.



Step 12: Start the Visualizer	
User	**Explanation**
a. From the Visualizer Control Panel menu bar window, click on **Start Visualizer**. **b.** Set the **Isometric View** orientation and **Normalize** the view. **c.** Click on **Volume Visualization** (**E** icon) along the top of the Visualizer window. **d.** From the Visualizer menu bar, click on *Edit > Edit MBIF*. **e.** Click on *Active Fields*. **f.** Check the *Mass Fraction 1*, *Mass Fraction 2*, and *Mass Fraction 3* fields. **g.** **Update** and **Close** the window. **h.** In the Visualizer left panel, alternately select *Mass Fraction 1*, *Mass Fraction 2*, and *Mass Fraction 3*. **i.** View the results; see Figure 5-3 **j.** When finished, **Stop Visualizer**. **k.** Click on **Done** to close the hierarchical results window.	= The simulation is for a reaction of two species, while the product is the third species. Species 1 is dissolved in water and enters through the inlet. Species 2 enters by diffusion (or some other mechanism) through the porous top wall, where it has the maximum concentration of 0.1. The reaction occurs at the bottom wall, where there is a catalyst which causes the reactions to occur. If you look at the concentration profile of Species 2 it is maximum at the top twall and minimum at the bottom bwall. Also, there will be a reduction in Species 2 concentration moving downstream with the flow (and likewise for Species 1) while Species 3 (the product of the reaction, and selected as Scalar 1) will increase in concentration moving downstream.

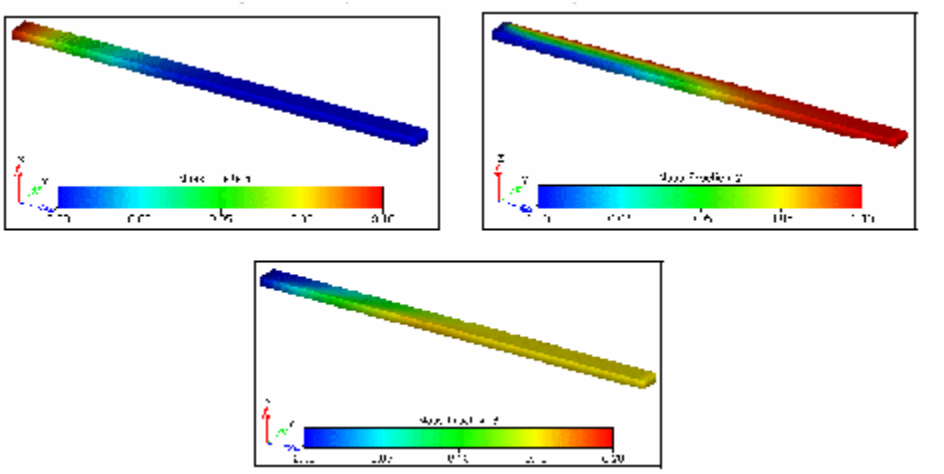
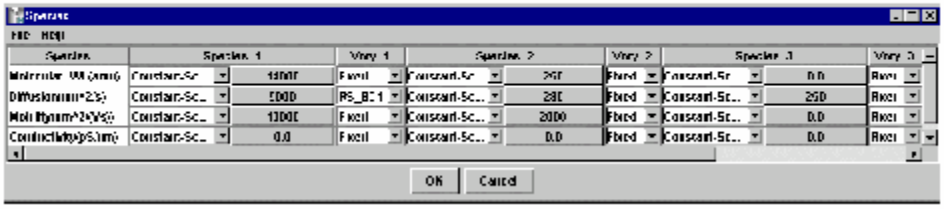


Figure 5-3 Species movement through the channel

5.2.4: ReactSim Preparation for SimMan

In this next sequence, you will investigate the effect of varying the diffusivity of the species in transport by using the Simulation Manager. In preparation, you'll need to change the boundary conditions to include a variable which can be assigned and for which a trajectory can be applied. While the ReactSim Model and Tool windows also must be con-figured, they should already be set if you are completing this tutorial sequentially.

Step 13: Set up and review ReactSim parameters	
User	**Explanation**
a. In the Analysis window, click on the **Solver Setup** button. **b.** Click on **Next** in the Tool window. **c.** From the ReactSim BCs window that appears, click on **Species**. **d.** On the Diffusion line for Species_1, change the Vary_1 column from *Fixed* to *RS_BC1*. **e.** Click on **OK**. **f.** Click on **Cancel** in the ReactSim BCs window.	- You are modifying the diffusivity for SimMan, and will use the *5000* setting as a trajectory incremental value. - You need to *Cancel* when finished because simulation control is through the Simulation Manager. However, your settings are still saved.



5.2.5: SimMan

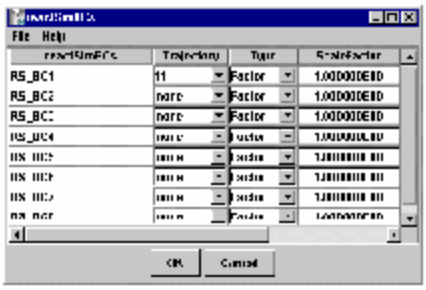
The remainder of the setup uses SimMan.

Step 14: Set up SimMan Model window	
User	**Explanation**
a. In the Analysis window, select *Managed Simulation* from the *Category* pull-down menu. **b.** Select *SimMan* from the *Type* pull-down menu. **c.** Set the *Input Mesh* file path to the same *channelr.mbif* file you have been using. **d.** Set the *Execution Mode* to *Interactive*. **e.** Create a solutions directory in the *ReactSim/Solutions* path to store the solver results. Name it *sm_run1*. **f.** Click on **Solver Setup**.	- The solver uses this window for path information.

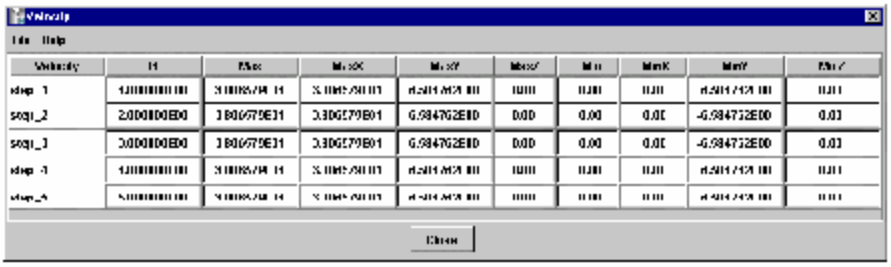
Step 15: Set up SimMan Tool window	
User	**Explanation**
a. In the SimMan Tool window set the solver to *ReactSim*. **b.** Click on **Next**.	– The Simulation Manager uses ReactSim to compute a solution for the trajectory sequence that will be run.

Step 16: Set the SimMan trajectory	
User	**Explanation**
a. In the SimMan BCs Settings window that opens, click on the **trajectory** button. **b.** Set the t1 Trajectory Type to *Delta*. **c.** Click on **Edit**. **d.** In the Edit Delta window, set the increment values as shown below. **e.** Click on **OK**. **f.** In the label column for t1, delete "t1" and type "Diffusion." **g.** Click on **OK**.	– The diffusion is varied from 5000 to 25000 in 5 steps. – You're setting the values so the Simulation Manager runs 5 sets of computations. – The Label column places a user-defined label as the abscissa annotation.

Step 17: Assign the ReactSim variable	
User	**Explanation**
a. Click on the **rsSimBCs** button. **b.** Set the RS_BC1 line trajectory to *t1*. **c.** Click on **OK**. **d.** Click on **Simulate**	– The t1 trajectory is assigned to the *RS_BC1* variable tagged in the Species window.The simulation starts. When finished, a Simulation Results window appears



Step 18: View the SimMan results	
User	**Explanation**
– Click on **Velocity Table** to view the simulation results. – View the results. a. Close the windows.	– The table shows the five trajectory steps, with increasing 5000 increments. The velocity does not change as a function of diffusion.



Step 19: Start the Visualizer / review results	
User	**Explanation**
a. From the Visualizer Control Panel menu bar window, click on **Start Visualizer**. **b.** Click on **Visualize List**. **c.** Click on the **Isometric View** button. **d.** Click on **Volume Visualization**. **e.** Review the *Mass Fraction 1*, *Mass Fraction 2*, and *Scalar 1* results. **f.** Stop Visualizer. **g.** In the simulation results window, click on **Done**.	– The complete matrix of 5 steps for each of the three parameter views is shown in Figure 5-4. – You're finished with this tutorial segment.

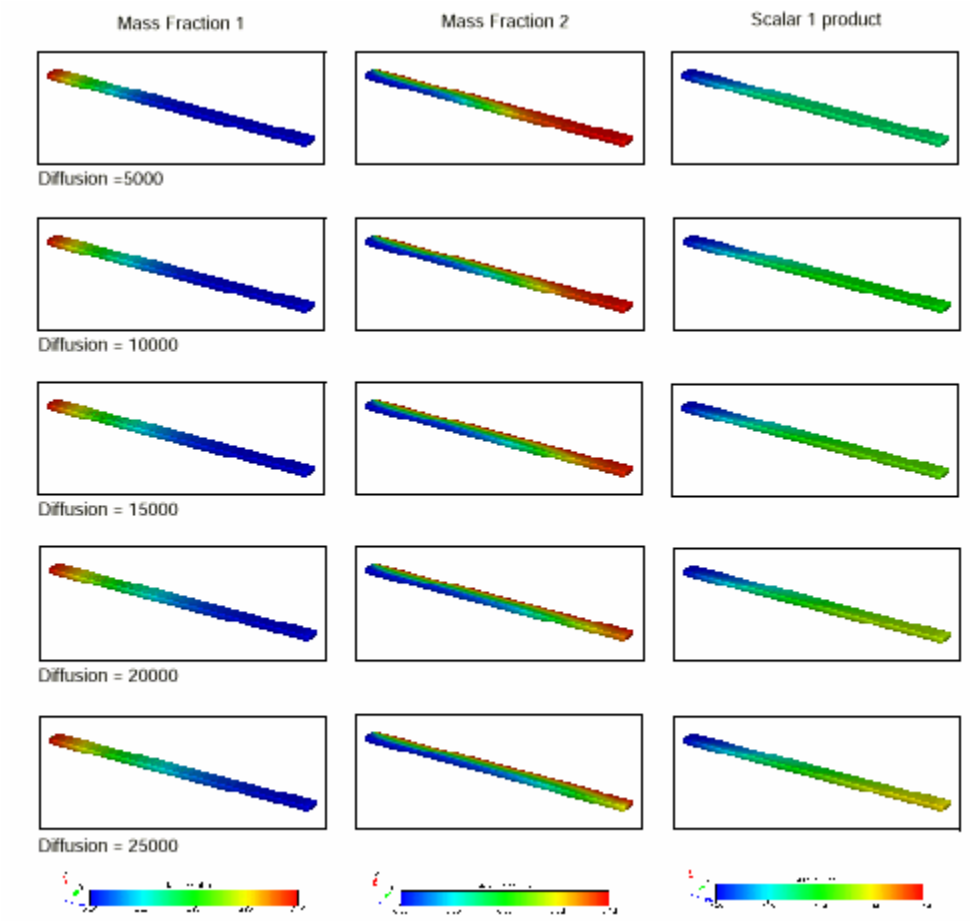


Figure 5-4 Mass Fraction and Scalar Results as a Function of Diffusion

5.3: Reference

This section explains the ReactSim windows and the setting options available. The window map in Figure 5-5 is an overview of the ReactSim solver flow.

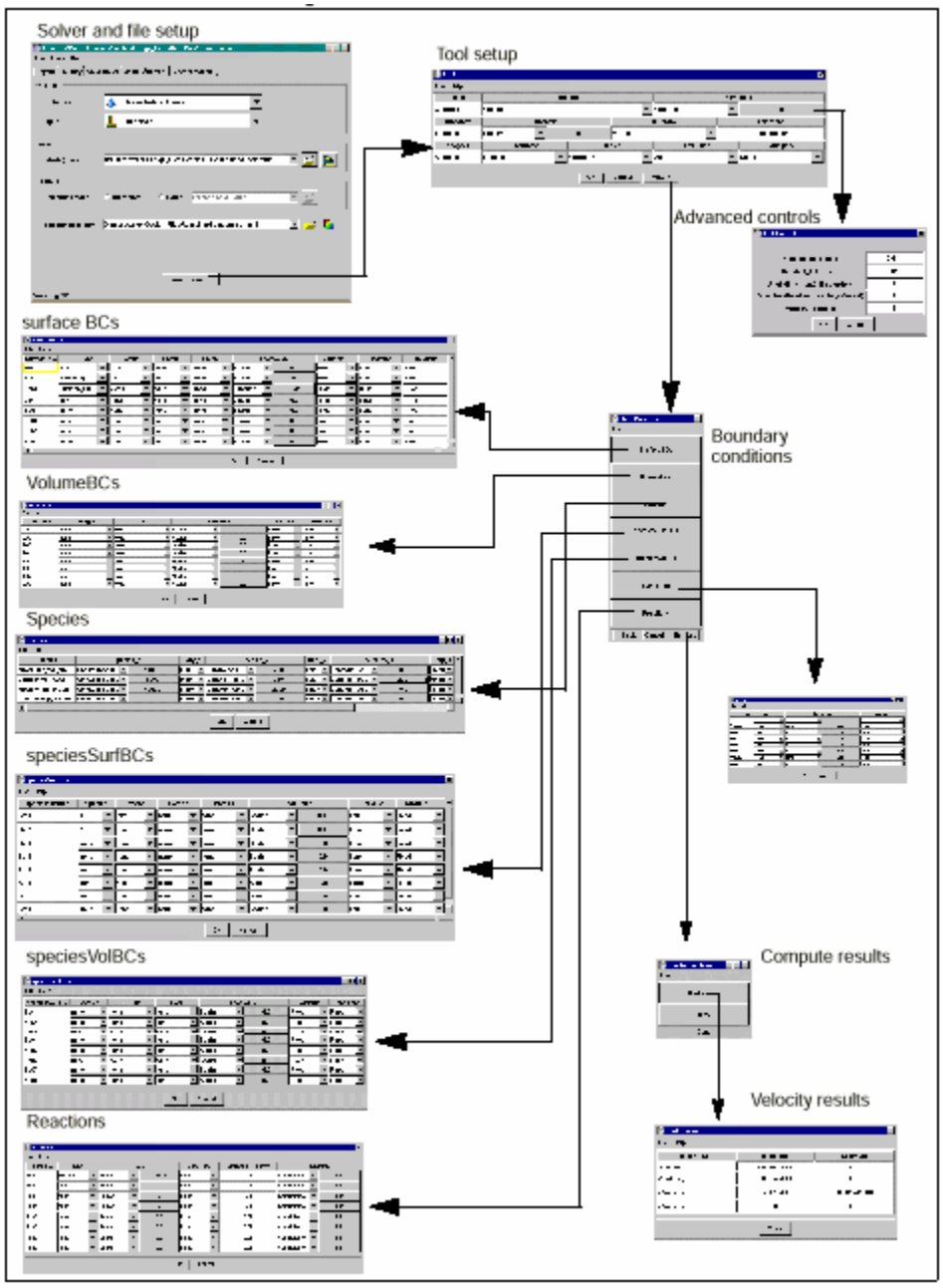
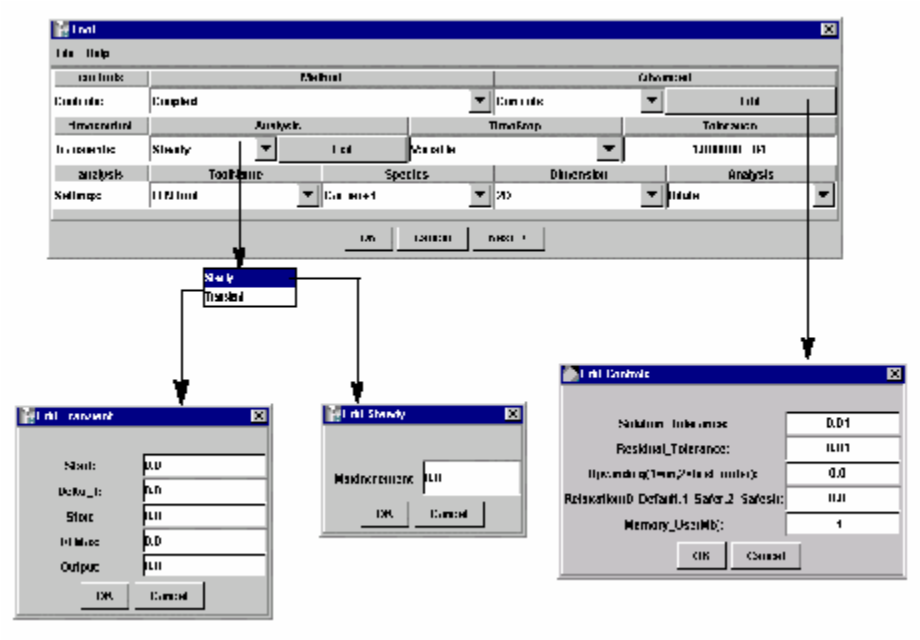


Figure 5-5 ReactSim Solver Flow

5.3.1: Tool Window

The Tool window allows the user to set parameters for running the ReactSim solver. Most of the information in the tool window provides the instructions to ReactSim. For fluidics, an important setting illustrated in the tutorials is the choice of solving as a 2-D, 2-D-axisymmetric, or 3-D problem.



Controls/Method

The Navier-Stokes equations used in the ReactSim solvers are non-linear and require an iterative approach to solving problems. The solvers adjust a variety of variables as part of the solution method, allowing them to solve both straightforward problems with single solutions, as well as more complex problems with multiple local minimum or maximum values.

- **Coupled**: The coupled solver is the default choice for ReactSim. This iterative solver is recommended for most problems, and can handle steady state and transient flows.
- **Segregated**: The segregated solver solves each degree of freedom in the problem separately and consecutively. Thus, the three momentum equations for flow in the X, Y, and Z directions and the pressure and energy equations are each solved separately. This approach uses less system memory at the expense of a longer solution time. It is recommended for problems containing more than 2500 elements.

Controls/Advanced Controls

Several different tolerances may be set depending on the non-linearity of the ReactSim flow problem.

- **Solution Tolerance**: This parameter is used to set the convergence criteria for the solution vector. It is defined as the norm of the change in the solution vector. For the coupled solvers the residual tolerance is also checked to determine convergence. For large problems, the default value of 0.01 will ensure a solution in a reasonable time. For smaller problems this value may be decreased even further.

- **Residual Tolerance**: The residual tolerance sets the convergence criterion for the norm of the residual force vector. The change in the force vector needs to be below this number for convergence.
- **Upwinding**: The upwinding parameter controls the addition of streamwise upwinding (tensor diffusion) to the various equations. The additional diffusion is generally useful in stabilizing the solution and preventing over/undershoots in time integration. The value of the upwinding parameter can be 0, 1, or 2. A value of 0 specifies no upwinding, a value of 1 switches upwinding on, and a value of 2 is first order.
- **Relaxation**: Specifies relaxation factors for the degrees of freedom in the system. The value of 0 is the default relaxation setting and is recommended for most solutions. The value of 1 is a more conservative setting, recommended for more difficult solutions such as a high Reynolds number or a high Peclet number. The value of 2 is the most conservative and is recommended for solutions that diverge when using the first two options. Optimal values are problem-dependent, and can be derived only by trial and error.
- **Memory Use**: The default setting is -1, which allows the software to allocate memory as required. For large 3-D problems, or to avoid unnecessary swapping, the user should set this value if the job is much bigger than the RAM memory. A suggested range is 2/3 to 4/5 of actual RAM.

Transients/Analysis

- **Steady:** Performs a steady state, or time-independent, analysis. The solver will try and converge to an answer within the number of steps given in the Edit window MaxIncrement setting.
- **Transient:** This setting sets up the transient simulation. Five time steps are set:

  Start: Time to start simulation.
  Delta_T: Time interval for simulation. It should be set to a very small number, about 1e-6 times the Stop value if variable time step is used.
  Stop: Time to stop simulation.
  DTMax: When TimeStep is set to Variable, sets the maximum range for the time step. If set to 0, it is ignored. It should be set to 0, except for complex problems, where it should be set to 1/100 of the total simulation time (0.01* (Stop - Start)).
  Output: Specify time increments at which the mbif files are written. For example, a setting of 0.2 writes an mbif file every 0.2 seconds for the duration of the simulation.

Transients/TimeStep

This controls the time step of the overall transient analysis.

- **Variable**: This time stepping control default value is the optimal setting. The solver determines the time step value at any given point in the solution. With a variable setting, the solver can use small time steps at the beginning of the problem, and larger steps near the end when the solution is nearly complete.
- **Fixed**: This time step is used for special problems. An example is when the solver would increase the timestep in the variable mode with steps that are larger than the time in which the effects that are studied occur. In highly viscous flows the actual startup effects of the flow might be skipped.

Transients/Tolerance

Tolerance allows the specification of the local truncation error (convergence) within each time step in the transient analysis. In general, the solver iterates to this convergence limit at each time step before continuing. Examining the mass conservation plot at the end of a transient simulation may check the accuracy of the solution. Depending on the mass conservation plot results, the Tolerance value may be decreased from the default setting of 0.001.

Analysis Settings/Tool name

- **FEMTool**: The FEMTool uses the Fidap solver. Fidap uses parabolic finite elements, and is more accurate for coarse meshes.

Analysis Settings/Species

Refers to the total number of components present in the flow. ReactSim supports up to 4 additional reaction species in addition to the carrier fluid. Choices are Carrier+2, Carrier+3, or Carrier+4.

Analysis Settings/Dimension

- **3D**: Tells the solver to run a three dimensional solution with dimensions X,Y, and Z.
- **2D-Axi**: Allows the user to run a two dimensional axi-symmetric solution. The model has to be generated in the XY-plane and should be 1 element thick in the Z direction. The X-axis is the axis of symmetry and the Y-axis is the radial coordinate.
- **2D**: allows the user to run a two dimensional solution. The model has to be generated in the XY-plane and should be 1 element thick in the Z direction. No boundary conditions may be applied to surfaces which lie in this X-Y plane.

Analysis Settings/Analysis

Sets the type of analysis to be performed, depending on the concentration of the fluid. Dilute and Non-Dilute are the choices.

OK

Applies changes to the window, but does not continue with ReactSim. Control returns to the Analysis tab window.

Cancel

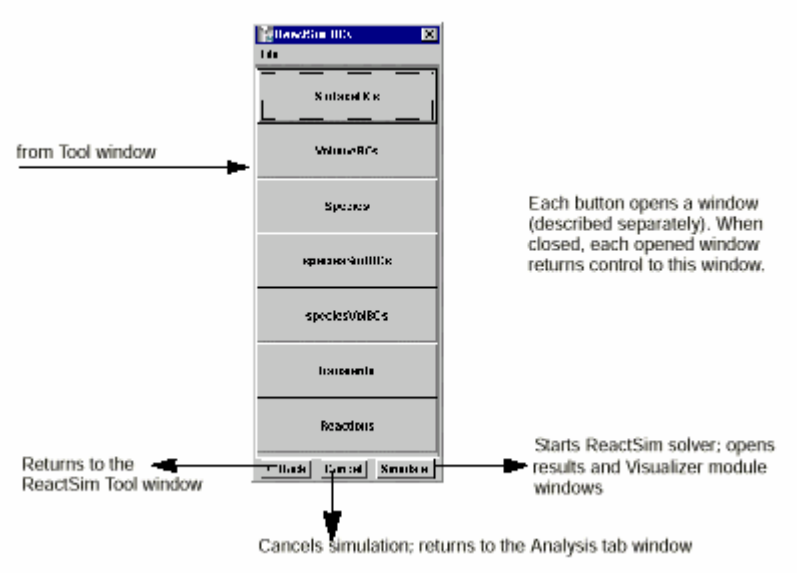
Does not apply changes to the window. Control returns to the Analysis tab window.

Next

Applies changes to the window; opens the ReactSim boundary conditions window.

5.3.2: ReactSim Boundary Conditions Window

The ReactSim BCs hierarchical boundary conditions menu window allows user to choose windows to specify load conditions for the ReactSim fluidic solver.



SurfaceBCs

Opens window (see page 132) to set surface boundary conditions, such as velocity and pressure.

VolumeBCs

Opens window (see page 136) to set boundary conditions that affect an entire volume, such as temperature conditions.

Species

Opens a window to specify species characteristics.

speciesSurfBCs

Opens window (see page 140) to set species surface boundary conditions.

speciesVolBCs

Opens window to set species volume boundary conditions.

transients

Opens window to set conditions for transient calculations.

Reactions

Opens window to set conditions for the reaction.

Back

Closes the ReactSim BCs window, and returns to the ReactSim Tool window.

Cancel

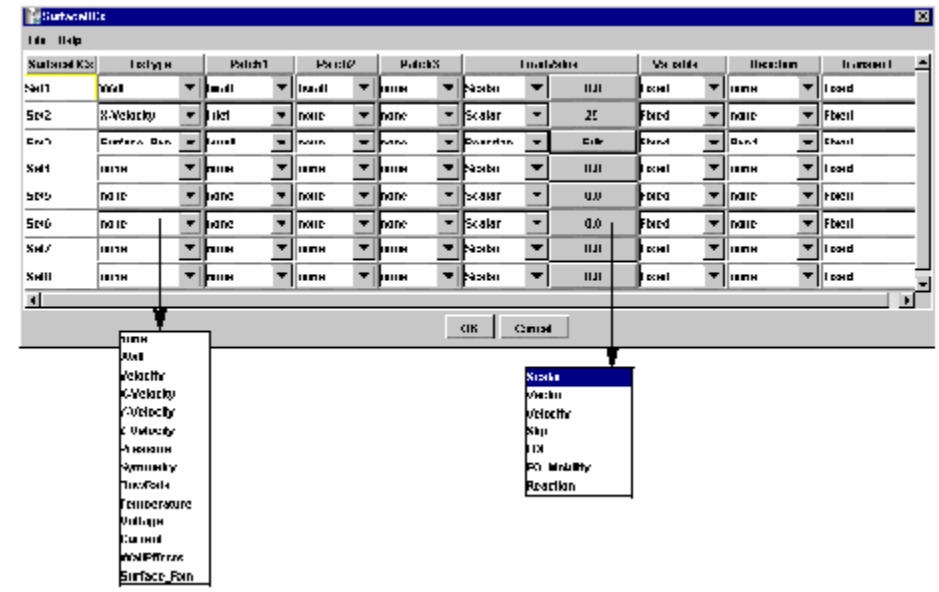
Does not proceed with ReactSim solver; returns to Analysis tab window.

Simulate

Launches ReactSim solver.

Surface Boundary Conditions Window

The SurfaceBCs window sets patch surface boundary conditions. Fix types and load conditions for these surfaces can be specified in eight sets within this window. When setting up conditions, the LoadValue button needs to correspond to the appropriate boundary condition. Not all combinations of boundary conditions and LoadValues are possible.



SurfaceBCs

This display-only column allows the user to define up to eight boundary condition sets for the model.

Fix Type

Enables pull-down menu with many load type choices:

- **Wall**: This represents a “no slip” (zero velocity) boundary condition at the selected patches. The no-slip boundary condition is an assumption that is made in Newtonian Fluids. No LoadValue is applied.
- **Velocity**: Velocity is set at a patch. The specification is in the form of a quadratic polynomial in all three directions. For each velocity component, a separate polynomial can be provided. Use with Velocity Load-Value.

- **X-Velocity**: This option specifies the X-component of velocity to uniform value. The option is very useful when applying symmetric boundary conditions for which the velocity perpendicular to the axis of symmetry is 0. A Scalar LoadValue is used.

- **Y-Velocity**: This option specifies the Y-component of velocity to uniform value. The option is very useful when applying symmetric boundary conditions for which the velocity perpendicular to the axis of symmetry is 0. A Scalar LoadValue is used.

- **Z-Velocity**: This option specifies the Z-component of velocity to uniform value. The option is very useful when applying symmetric boundary conditions for which the velocity perpendicular to the axis of symmetry is 0. A Scalar LoadValue is used.

- **Pressure**: A constant pressure on the selected patch is specified. The pressure is input as a normal stress to the computation. A Scalar LoadValue is used.

- **Symmetry**: The selected patch is a plane of symmetry — all fluxes normal to this plane are zero, as is the normal velocity component. It is important that the problem is symmetrical and not just the geometry. In general, it is more efficient to use the X-, Y-, and Z-Velocity settings to apply symmetry if the plane is parallel to any of the axis planes. No LoadValue is applied.

- **MassFlux**: A Vector LoadValue is used.

- **FlowRate**: The flow rate follows the sign convention of all boundary conditions. A positive flow rate is along the normal of the selected patch. Because the normal always points to the volume in Coventor software, the FlowRate is into the patch when a positive value is specified. A Scalar LoadValue is used.

- **Temperature**: Applies a constant temperature on the selected patch. A Scalar LoadValue is used. Units are in Kelvin.

- **Voltage**: This boundary condition applies a constant potential on the specified patch. Note that a potential difference must be specified; therefore, two Voltage BC specifications are required. A Scalar LoadValue is used.

- **Current**: This boundary condition applies a current through the specified patch. A Scalar LoadValue is used.

- **Wall Effects**: This boundary condition allows the specification of electroosmotic effects in the flow. EO_Mobility and Slip LoadValues can be used.

- **Surface_Rxn**: Sets the surface at which the reaction occurs. The Reaction LoadValue is applied (with no value). A reaction variable can be assigned on this line and defined in the Reactions window.

Patch1,2,3r

Choose from any of the patch names previously set up.

Load Value

Choose from several load types. Each type uses a different edit window; the entire set of edit windows is shown as part of the LoadValue explanation.

- **Scalar**: one-dimensional quantity, such as pressure load or temperature.

- **Vector:** Used with the Velocity FixType. This defines a uniform velocity profile in the direction of the x, y, or z vector specified on the selected patch.

- Velocity: Used with the Velocity FixType. This is a quadratic, linear or constant polynomial in all three directions for the velocity on the selected patch. For each velocity U_x, U_y, and U_z a separate polynomial can be given. For example, Pouiselle Flow in a pipe yields the following profile:

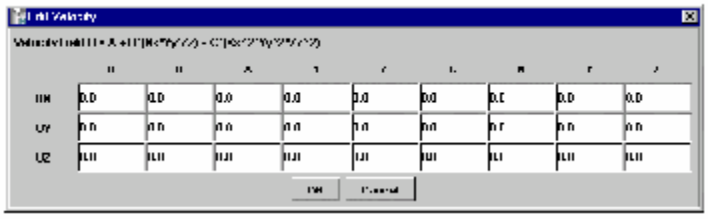
$$U = C\left[1 - \left(\frac{Y}{Y_0}\right)^2\right]$$

where C is a constant and Y_0 is the pipe radius.

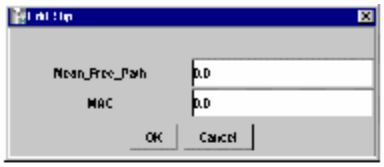
For this example, the Edit Velocity window below requires that only the first U_x line needs to be filled in. The following column values are required for this window:

Column $A = C$, Column $C = -C$, Column $Y_y^2 = 1$. All remaining columns are zero.

The example shown is filled out for the constant $C = 5$.



Slip: Used with the Wall Effects FixType. The Mean Free Path and the MAC (Momentum Accommodation Coefficient) are used in the slip equation to study wall effects in microchannels.



The slip velocity at the wall can be expressed as follows:

$$SlipVelocity = \sigma K\left(\frac{\partial U}{\partial n}\right)_{wall}$$

where U is the velocity, n is the direction normal to the velocity, σ is the streamwise momentum accommodation, expressed as follows:

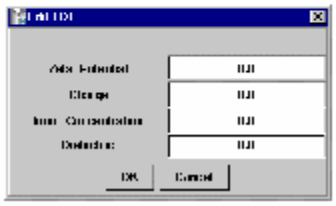
$$\sigma = \frac{2 - \sigma_m}{\sigma_m}$$

where σ_m is the momentum accommodation coefficient (MAC). Usually, $\sigma_m = 1$ but it can vary within the range $0 < \sigma_m < 1$.

K is the Knudsen number, which can be expressed as:

$$K_n = \frac{MeanFreePath}{CharacteristicLength}$$

If this value is smaller than 0.01 the slip effect is neglected.



- EO_Mobility: Used with the Wall Effects FixType. This setting enables the representation of the electroosmotic effects on the walls through a mobility that defines the velocity achieved by the charged carrier at the edge of the double layer in the electric field. Note that this implies a relaxation of the no-slip wall boundary condition, since the near- wall region is no longer solved. The EO_Mobility is a positive number for a negatively charged wall. (In other words, a positive value will result in flow towards the negative electrode.)

- Reaction: Used with the Surface_Rxn FixType. No setup or LoadValue window is used.

Variable

Setting for Simulation Manager. A Fixed Variable setting (the default) uses constant Load Values, which are not changed during a Simulation Manager run. When a Load Value is to be a variable modified by a Simulation Manager trajectory, one of eight RS_BC variables can be used, corresponding to the lines in the rsSimBCs Simulation Manager setup window.

Reaction

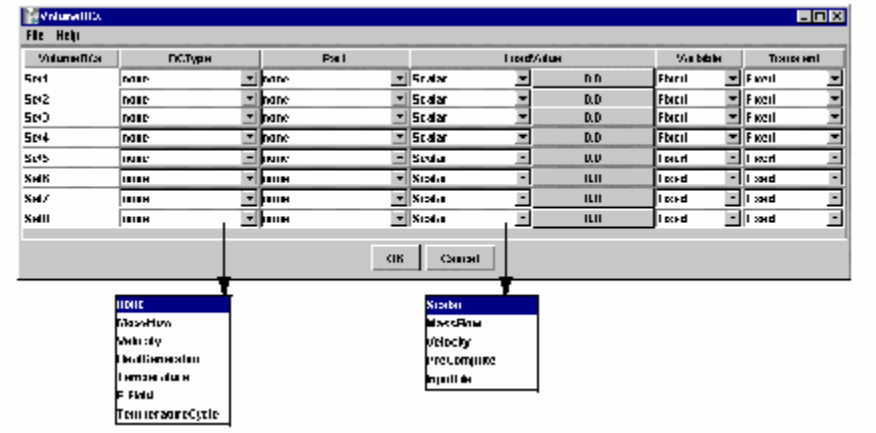
Sets the reaction type variable. Choices are Rxn1 through Rxn8. The reaction variable that is assigned is defined in the Reactions window.

Transient

Setting for transients surface boundary condition. A Fixed Transient setting (the default) does not apply transients. When a Set is to be modified by a transient event, one of two Transient variables are available for assignment. The variable is defined in the transients window. With this technique a periodic pressure or input flow can be generated. By setting the Transient variable the input on that node set is coupled to the waves or function defined in the transients window.

ReactSim Volume Boundary Conditions Window

The VolumeBCs window sets volume boundary conditions. Types and load conditions for these volumes can be specified in Part sets within this window.



VolumeBCs

This display-only column allows the user to define up to eight boundary condition sets for the model.

BCType

Enables pull-down menu with several choices:

- **none**: Does not apply a boundary condition to the volume.
- **MassFlow**: Specifies a mass flow in three directions—Mx, My, Mz. The Mass Flow LoadValue is used.
- **Velocity**: Applies a velocity to separate or decouple the species calculation from the flow calculation. The setting is valid only if the species flow does not influence the carrier fluid flow. A Velocity, PreCompute, or InputFile LoadValue is used.
- **Heat Generation**: Heat can be generated in a part. The part is usually a solid and not a fluid. A Scalar Load-Value is used.
- **Temperature**: Applies a fixed temperature to the selected part. A Scalar LoadValue is used.
- **E-Field**: The E-Field in the volume can be read from a pre-computed mbif file. An InputFile LoadValue is used.
- **Temperature Cycle**: Applies a temperature cycle to the part. A Scalar LoadValue is used.

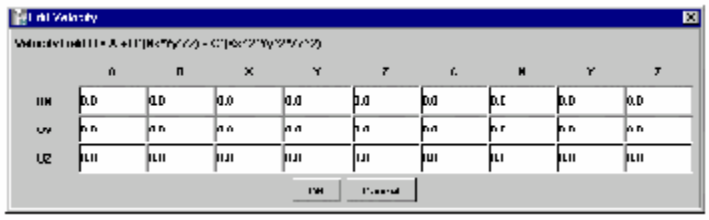
Part
Enables pull-down menu with a list of all the parts modeled and stored in the mbif file.

Load Value
Choose from several load types. Each type uses a different edit window, shown below with the LoadValue description.

- **Scalar**: Used to specify a one-dimensional value, such as Temperature or Heat Generation.

- **Mass Flow**: Used to specify a three-dimensional value for Mass Flow.

- **Velocity**: Used with the Velocity BCType. This is a quadratic, linear or constant polynomial in all three directions applying a uniform velocity profile on the selected part. For each velocity U_x, U_y, and U_z a separate polynomial can be given.



- **PreCompute**: Decouples the momentum and species equations. The velocity is pre-computed and an advection-diffusion analysis for the species follows. No LoadValue edit window is used.

- **Input File**: Specifies a result mbif file from another simulation as the source data input initial conditions. The default directory is the directory from which the software is launched.

Variable

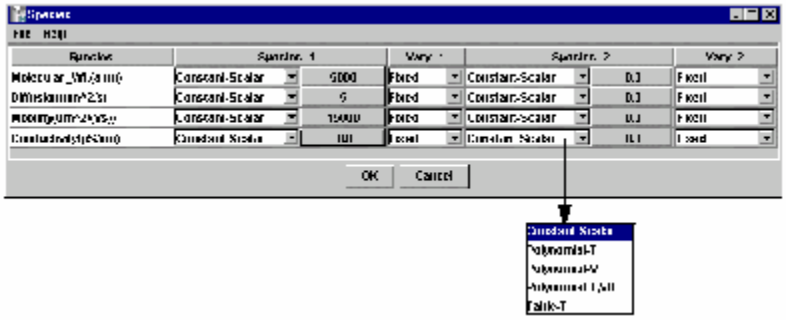
Setting for Simulation Manager. A Fixed Variable setting (the default) uses constant Load Values, which are not changed during a Simulation Manager run. When a Load Value is to be a variable modified by a Simulation Manager trajectory, one of eight RS_BC variables can be used, corresponding to the lines in the rsSimBCs Simulation Manager setup window.

Transient

Setting for transients volume boundary condition. A Fixed Transient setting (the default) does not apply transients. When a Part is to be modified by a transient event, one of two Transient variables are available for assignment. The variable is defined in the transients window.

Species Window

The Species window allows the user to specify the species characteristics used for the simulation. The species present are in infinitely dilute form, therefore material properties are not needed. The Tool window Species options are Carrier+2, Carrier+3, or Carrier+4. If set to Carrier+2, a two-column window appears. If set to Carrier+3, a three-column window appears. If set to Carrier+4, a four-column window appears.



Species

This view-only window lists the species parameters that user can specify for simulation: Molecular Weight, Diffusion, Mobility, and Conductivity.

Species_1, Species_2

Designates the type of parameter to be specified. Choices include:

- **Constant-Scalar**: Constant with a single value over the entire field.
- **Polynomial-T**: Polynomial function of temperature. Six constant coefficients are allowed to enable the definition of up to a fifth order polynomial.
- **Polynomial-V**: Solves for non-linear electrophoresis. The user enters up to six polynomial coefficients.

  For non-linear electrophoresis problems where the electrophoretic mobility changes significantly, oscillations may be observed in the solution. These can be damped out by turning on Upwinding (from the Advanced button in the Tool window) and setting the value to 1. After running a simulation, the user should check the spIntegral results table carefully. It may be necessary to adjust the Tool window Timestep to Variable, and the Tolerance value downwards (in the range of 1.0e-03 to 1.0e-06) to improve mass conservation.

- **Polynomial-T,V0**: Polynomial function of temperature, with the V_0 term used to define an initial start-up voltage below which electrophoretic effects are absent.
- **Table-T**: Tabular form for defining temperature-property pairs. Linear interpolation is used for intermediate values.

Edit window

Specifies the parameter value in this window. Window format dependent on the parameter type specified. The Edit window are shown on page 139.

Vary_1, Vary_2

Allows specification of a variable tag for Simulation Manager runs.

Species Edit Windows

Each LoadValue type selected from the Species window uses its own format for entering parameters. The windows are described in more detail in this section.

Constant-Scalar

Constant with a single value over the entire field.

Polynomial-T

Polynomial function of temperature. Six constant coefficients are allowed to enable the definition of up to a fifth order polynomial.

Polynomial-V

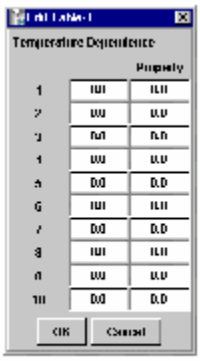
Polynomial function of electric field strength. Used to calculate non-linear electrophoresis. The user enters up to six polynomial coefficients.

Polynomial-T,V0

Polynomial function of temperature, with the V_0 term used to define an initial start-up voltage below which electrophoretic effects are absent.

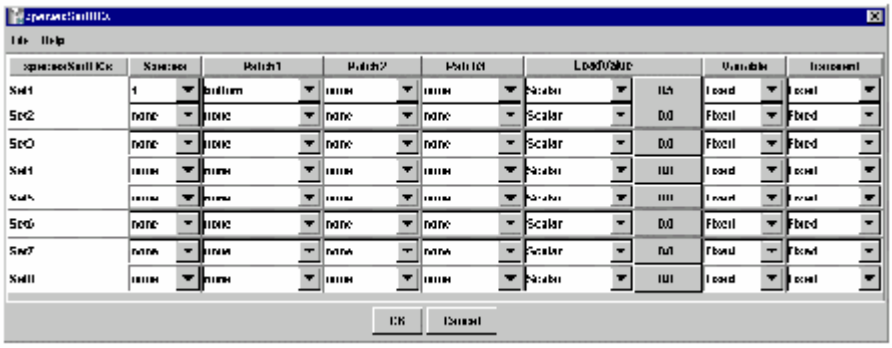
Table-T

Tabular form for defining temperature-property pairs. Linear interpolation is used for intermediate values.



Species Surface Boundary Conditions Window

The speciesSurfBCs window sets surface boundary conditions for the species. Fix types and load conditions for these surfaces can be specified in eight sets within this window. When setting conditions, the LoadValue button has to correspond to the appropriate boundary condition. Not all combinations of species settings and LoadValues are possible.



speciesSurfBCs

This display-only column allows the user to define up to eight boundary condition sets for the model.

Species

Can choose any of 3 species for the setting.

Patch1,2,3

Choose from any of the patch names previously set up.

Load Value

Choose from several load types. Each type uses a different edit window; the entire set of edit windows is shown as part of the LoadValue explanation.

- **Scalar**: a fixed value on a patch.
- **Inj_Gaussian**: the injection of a finite width Gaussian plug through the patch. The Full-Width at Half Max (FWHM) value can be defined in seconds or in microns.

- **Inj_Plug**: the injection of a finite width square plug through the patch. The Length of the plug can be defined in seconds or in microns.

Variable

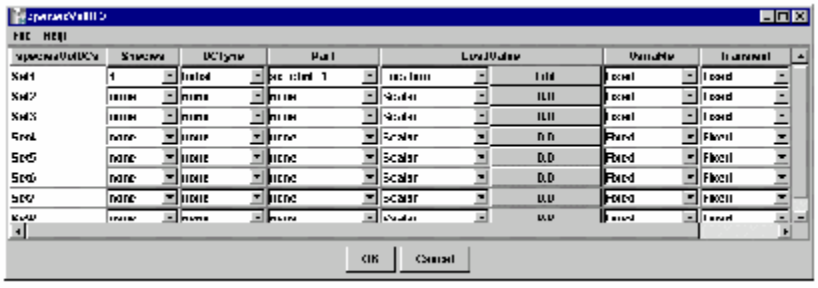
Setting for Simulation Manager. A Fixed setting (the default) uses constant Load Values, which are not changed during a Simulation Manager run. When a Load Value is to be a variable modified by a Simulation Manager trajectory, one of eight RS_BC variables can be used, corresponding to the lines in the rsSimBCs Simulation Manager setup window.

Transient

Setting for transients surface boundary condition. A Fixed setting (the default) does not apply transients. When a set is to be modified by a transient event, one of two Transient variables are available for assignment. The variable is defined in the transients window. With this technique a periodic pressure or input flow can be generated. By setting the Transient variable the input on that node set is coupled to the waves or function defined in the transients window.

Species Volume Boundary Conditions Window

The speciesVolBCs window sets volume boundary conditions for the species. Types and load conditions for these volumes can be specified in Part sets within this window.



speciesVolBCs

This display-only column allows the user to define up to eight boundary condition sets for the model.

Species

Can choose one of 3 species for the setting.

BCType

Enables pull-down menu with several choices:

- **none**: does not apply a boundary condition to the volume.
- **Fixed**: fixes the selected volume.
- **Initial**: This boundary condition is used only for transient flow analysis. A patch needs to be associated and selected in order to pose a numerically correct problem. The selected method enters Mass Fraction into the flow as desired. The transient problem needs a Dirichlet BC for the concentration, which is chosen to be 0 on the selected patch. Thus, the selected patch should be far enough upstream in order for the Mass Fraction not to reach the patch at any time.

Part

Enables pull-down menu with a list of all the parts modeled and stored in the mbif file.

Load Value

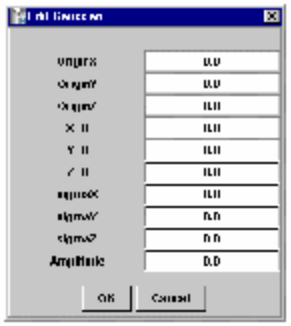
Choose from several load types. Each type uses a different edit window, shown below with the LoadValue description.

- **Scalar**: Used to specify a one-dimensional value, such as Temperature or Heat Generation.
- **Location**: Confines the concentration, given by the Mass Fraction, to the selected minimum and maximum values of X, Y, and Z. Coventor software finds all nodes that are within these bounds and applies the Mass Fraction. If the minimum and maximum in any direction are left unchanged (i.e zero), it means that "no filter" (all elements between - _ and + __) is applied in this direction. Using this LoadValue can lead to solver uncertainties, due to the sharp edges created by the Location setting. The Gaussian setting is preferred.

- **Gaussian**: Applies a Gaussian distribution according to the following formula:

$$A\exp\left[\left(\frac{X-X_0}{\sigma_x}\right)^2\right]\left[\left(\frac{Y-Y_0}{\sigma_y}\right)^2\right]\left[\left(\frac{Z-Z_0}{\sigma_z}\right)^2\right]$$

where A is the amplitude, and σ is the change in a particular direction. Typically, only one dimension is given a non-zero σ value, which results in a species plug with a Gaussian distribution in one axial direction. The Gaussian setting greatly reduces solver instability, and is the preferred LoadValue for most calculations.



- **Input File**: Specifies a result mbif file from another simulation as the source data input boundary conditions. The default directory is the directory from which the software is launched.

Variable

Setting for Simulation Manager. A Fixed setting (the default) uses constant Load Values, which are not changed during a Simulation Manager run. When a Load Value is to be a variable modified by a Simulation Manager trajectory, one of eight RS_BC variables can be used, corresponding to the lines in the rsSimBCs Simulation Manager setup window.

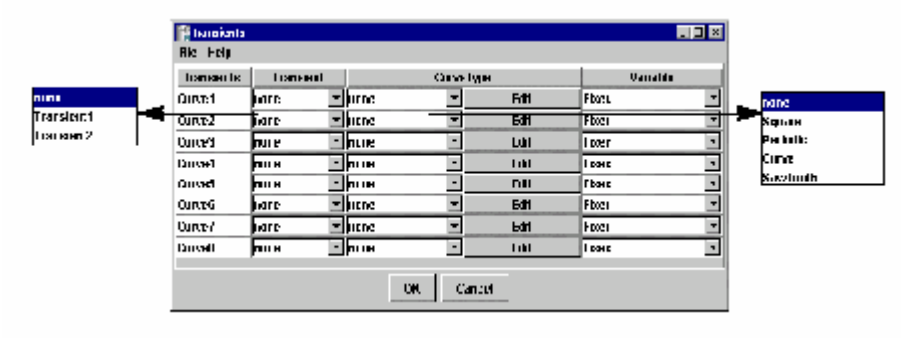
Transient

Setting for transients surface boundary condition. A Fixed setting (the default) does not apply transients. When a Set is to be modified by a transient event, one of two Transient variables are available for assignment. The variable is defined in the transients window.

Transients Boundary Conditions Window

The transients window enables the user to specify boundary conditions associated with transient calculations. Transient variables can be assigned in the SurfaceBCs or VolumeBCs window, and the type of transient response to use for the problem can be specified in this window. Two different transient types can be specified. For any transient analysis, the appropriate parameters should be set up in the ReactSim Tool window.

Transients are restricted to the following boundary condition settings: SurfaceBCs—Velocity, X,Y,Z Velocity, Pressure, FlowRate Temperature, Heat Flux, Concentration; VolumeBCs—Heat Generation.



transients

This display-only column allow the user to define up to eight boundary condition transient sets for the model.

Transient

This column allows assignment of one of two transient curve variables: Transient1 or Transient2. The equivalent TransientBC1 and TransientBC2 variables are assigned in either the SurfaceBC or VolumeBC window to a desired parameter for transient analysis.

Curve Type / Edit

The ReactSim transient capability allows one of four different transient waveforms to be specified for the analysis. The specific waveform characteristics are specified in the Edit window accessed from the Edit button. These Edit windows are further described on page 145.

- **Square**: Assigns a square wave as the transient curve. The square wave can be controlled by adjusting its period, split (duty cycle), or amplitude.
- **Periodic**: Assigns a periodic curve as the transient. The periodic curve can be controlled by adjusting its period, mean, or amplitude.
- **Curve**: Assigns a table of time step and property values in order to create a customized curve.
- **Sawtooth**: Produces a sawtooth waveform.

Variable

Setting for Simulation Manager. A Fixed setting (the default) uses constant Load Values, which are not changed during a Simulation Manager run. When a Load Value is to be a variable modified by a Simulation Manager trajectory, one of two FluidBC variables can be used, corresponding to the lines in the fluidBCs Simulation Manager setup window.

Transients BC Edit CurveType Windows

Each transient LoadValue type selected from the Edit CurveType window uses its own format for entering parameters. The windows are described in more detail in this section.

Square

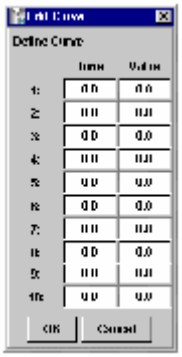
The square wave can be controlled by adjusting its period, split (duty cycle), or amplitude. Period is the time between the start of two square waves. Split is a value between 0 and 1. If Split is 0.5, the square wave is at its maximum for half a period. If the Split is 0.3, then the square wave is at its maximum for 30% of the period. Amplitude is the maximum value of the square wave.

Periodic

The periodic wave can be controlled by adjusting its period, mean, or amplitude: Period is the time between the start of two periodic waves. Mean moves the periodic curve vertically (up or down). Amplitude is the maximum value of the periodic wave.

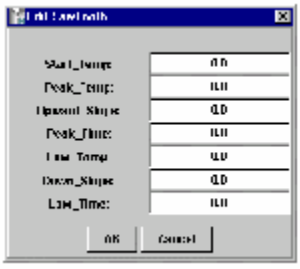
Curve

The custom curve is described with a table of time step and property values. Users can enter up to 10 different sets of time and amplitude values to simulate almost any type of transient curve.



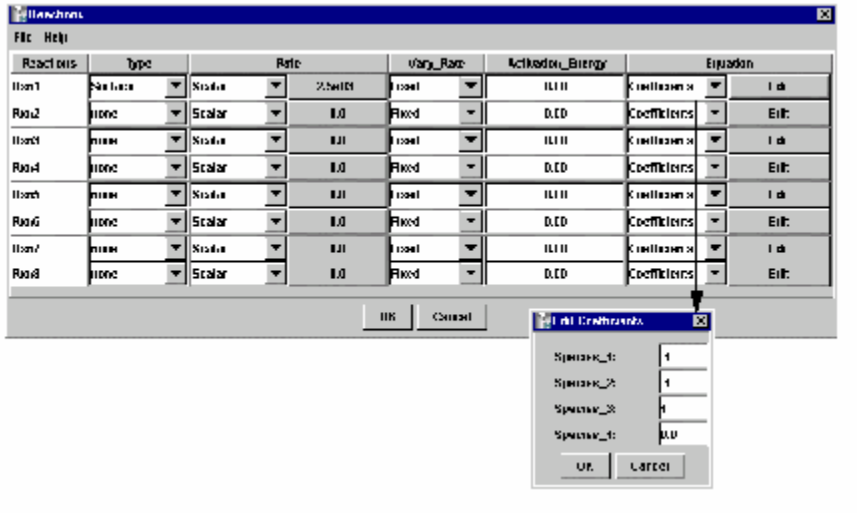
Sawtooth

The sawtooth is described with a combination of time and temperature values, along with a slope specification for the sawtooth angle.



Reactions Boundary Conditions Window

The Reactions window enables the user to specify boundary condition characteristics associated with the resultant species reaction.



Reactions

This display-only column allows the user to define up to eight boundary condition reaction sets for the model.

Type

Reaction type choices are Surface or Volume.

Rate / Edit

The reaction rate can be specified as Scalar or as k(T-To)^Texp. The rate is entered in the Edit window associated with the setting. (Texp is the exponent on T-To).

Vary_Rate

Specifies as Fixed or tag as a variable for SimMan trajectory assignment. Variable choices are RS_BC1 through RS_BC8.

Activation_Energy

Specifies the value if known.

Equation / Edit

Specifies Coefficients (only choice) and enter values in the Edit window associated with the setting. The reaction is of the form:

$$nA + mB = pC + qD$$

where the coefficients n,m,p, and q are specified. The reactants are entered as negative numbers, while the products are entered as positive numbers.

5.3.3: Simulation Results Window

The fluidic results hierarchical solutions menu window allows user to choose windows to view result tables and mbif file paths used during the computation.

fluidDomain

Opens window to display table of fluid results.

files

Opens window to display path to result mbif file.

Done

Closes window and returns control to the function manager.

File/Print

Enables printing of the individual window results to a single file. The text format file can be used to interface to other programs, such as Microsoft Excel. The file is located in the directory from which the software starts.

Fluid Solution Window

This fluidDomain window displays the results from the FEM solver.

fluidDomain

Lists the type of velocity for the solver solution. Maximum velocity as well as the individual X,Y, and Z components
are displayed.

Maximum

The maximum velocity calculated by the solver. The value shown is an absolute value.

Minimum

The minimum velocity calculated by the solver. The sign of the value is derived from the normal vector; a minimum value can represent maximum velocity. If the value in this column represents the maximum velocity for the model, the same value will appear in the Maximum column.

Close

Closes window.

Result Files Window

This files window displays the path to the result mbif file.

Base File

Lists the full path of the result mbif file created by ReactSim.

Result Directory

Lists the path of the directory that stores the result mbif file.

Close

Closes window.

Appendix 1: Publications

Optimization of Sample Injection Components in Electrokinetic Microfluidic Systems

Luc Bousse[1] **and Abdel Minalla**
Caliper Technologies Corp.
Manish Deshpande[2]**, Ken B. Greiner and John R. Gilbert**
Microcosm Technologies Inc.

Abstract

This paper presents experimental data, simulation tools (FlumeCAD), simulation results, and their use together to analyze and improve the designs of electrokinetic injection and switching components for microchemical fluidic systems.

Introduction

Electrokinetic microfluidic microsystems are powerful analytical tools for many applications, such as nucleic acid analysis, enzyme assays, and immunoassays [1-6]. Such systems have gained considerable importance as components in micron-scale integrated chemical/biochemical analysis or synthesis systems, also referred to as lab-on-a-chip. The basic "unit process" operations in these systems are sample injection, mixing, chemical reaction or modification, separation, and detection. Assembling a system of many "unit process" nodes requires one or more transport mechanisms to move sample and reagents through the "wires" of the system. Many of these systems rely on electrokinetic physics as their transport mechanism, although pressure and pneumatic applications have also been demonstrated. Complicated relationships exist between the microchannel geometries, the conditions under which the devices operate, and the behavior of the multi-component fluids transported in these channels. In the past researchers have been forced to use costly trial and error methods to understand and design such microfluidic systems.

CAD tools can be a valuable aid in the design of microfluidic systems. Numerical analyses provide significant insight into the fluid mechanics in these systems. They allow the extraction of material and flow properties that are generally not well documented, or that vary from application to application or from one manufacturing technology to another. Furthermore such tools help the designer to explore a much larger space of designs than is easily available from experiment, and do so in a quantitative way which enables the extraction of key parameters for improved or optimal operation of common microchemical system components.

In this paper we include experimental data from some electrokinetic injection and switching components, as well as matching simulations of those components. We then demonstrate the use of the simulation tools to generate virtual experiments to help the designer choose good or optimal settings for the pinch field during injection and good or optimal settings for the switching field in a switch component.

The simplest switching component is an intersection of two channels. Such intersections are surprisingly powerful tools that enable the definition of sample plugs at the picoliter level [2]; this in turn allows microfabricated electrokinetic systems to outperform their conventional counterparts by orders of magnitude [3]. The switching components are employed in separation and dispensing systems to inject the sample from the load channel to the separation channel. A typical system employing such switching components is presented in Figure 1, showing a microfluidic system fabricated by etching and bonding in glass.

The parameters that determine optimal injection include:

- the length of the sample injected, which defines the quality of a subsequent separation
- the amount injected (the higher it is, the easier detection is); and
- The electrophoretic bias, i.e. the dependence of the injected amount on the mobility of the injected species.

The number of parameters involved in defining a given

Figure 1 : On-chip analysis system showing network of interconnected channels etched in the substrate. The intersections of the channels form the injection locations.

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injection is large: the currents involved in each step; the length of each step; and the exact geometry of the intersection. It is difficult to explore this entire universe experimentally to optimize the desired properties, and computer modeling of the injection process is thus very useful. Here, we demonstrate the use of numerical modelling in the design of such components, using the electrokinetic switch as an example.

Simulations of electrokinetic flows have been reported in the literature for both electrophoretic [7,8] and electroosmotic [9-10] flows. In [9] and [10], simulations of pinched injection have been reported in channel intersections, demonstrating the application of electrical fields to position the species plug in the intersection, prior to switching. These analyses are 2D steady-state analyses with fixed field boundary conditions. In this paper we report on the use of a new analysis tool (FlumeCAD) capable of full 3D analysis of electrokinetic physics with transient species loading and boundary conditions. Qualitative comparisons with experiment show good agreement with simulations as presented below. Characterization of the device based on applied fields is then presented to demonstrate the extraction of simplified models that allow the selection of optimal field strengths for specific device performance.

Experimental setup and Measurements

Experimental data was obtained on polymer chips that contained channels with a cross section of 12 by 35 microns. The DNA sample was a øX174/HaeIII size marker at a concentration of 200 ng/µl, in a 200 mM TAPS buffer solution. A fluorescent intercalating dye (SYBR Green I) was used to allow detection of the double-stranded DNA. The sieving matrix used was a 1.3 % solution of an acrylamide-based polymer. We determined that electroosmotic flow in these conditions was negligible.

The chip design was a simple cross, with a reagent well at the end of each arm of the cross. Two such designs were present in a single chip, for a total of eight wells, in a chip of dimension 22.4 by 37 mm.

The chip is loaded with reagents and inserted into a holder containing platinum electrodes connected to an eight-channel high-voltage power supply. This power supply is capable of either voltage or current control for each of the channels. The chip is observed on an inverted fluorescent microscope, one of whose optical outputs is directed towards an intensified CCD camera for visualization. A computer-controlled script is used in each experiment to define the voltages or currents at each terminal, and the time during which they are applied.

Numerical Formulation

The basic equations describing the fluid motion are the Navier-Stokes equations with appropriate electromigratory flux terms to represent the effect of the applied electric field on the carrier and/or the charged species. The effect of the applied field can be divided into two fundamental components:

Electrophoresis: The basis for electrophoresis is the differential migration of the charged species ions relative to the carrier molecules under the application of the external field. The differential migration is primarily an effect of the difference in the net charge between the solvent and solute ions, although frictional effects may also have some relevance. The migration velocity of the charged species can be expressed in terms of the applied field strength as

$$V_{ep} = \mu_{ep} E \qquad [1]$$

where μ_{ep} is the electrophoretic mobility of the ion in the carrier species. It is important to note that in most cases the carrier does not move under electrophoresis.

Electroosmosis: Electroosmosis, in contrast, is a macroscopic phenomenon involving the pumping of a fluid through a channel under the application of the field. In most cases, walls in microchannels are characterized by the presence of surface charges. The charge may either be due to the property of the wall or by adsorption of the charged species from the buffer. In the presence of an electrolyte the surface charge density induces the formation of a double layer in the fluid by attracting oppositely charged ions from the electrolyte to the immediate vicinity of the wall. The application of the electric field exerts a force on the fluid, which is initially felt only within the double layer. As a result the fluid in the near vicinity of the wall starts to move. Due to the viscous forces the fluid in the center of the channel is also accelerated until the net velocity gradient in the radial direction is zero and the whole fluid in the channel moves at a constant velocity.

The determination of the electroosmotic flow field requires the solution of the Navier-Stokes equation. The electroosmotic effect is incorporated as a force the $\rho_e E$ in the momentum equation. Here ρ_e is the charge density and E is the electric field intensity. The electric field can be determined by the solution of the potential equation, under the effects of both the applied field and the zeta potential on the walls. Formally, the Debye- Hückel [11] treatment using the Gouy-Chapman [11] concept of a diffuse double layer can be employed to compute the zeta potential distribution from the Poisson-Boltzmann equation.

In practice, the accurate solution of the Poisson-Boltzmann equation requires the resolution of the double layer. In general, the double layer thickness is extremely small in comparison to the channel width. For example, under nominal conditions for a 50 micron channel containing water, the double layer thickness is of O(nm). Adequate resolution of scales of this order is not generally tractable and further simplification is necessary. The effect of the potential across the double layer (the zeta potential) is felt as a force on the fluid at the edge of the double layer, and can be applied as a boundary condition on the wall

$$V_{eo} = \mu_{eo} E \qquad [2]$$

Which is analogous to the equation for the electrophoretic velocity, Eq. [1]. The electroosmotic mobility can then also be extracted using an approach similar to the electrophoretic case.

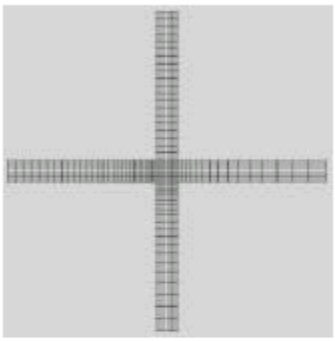

Figure 2 : Geometry of Intersection showing mesh over a slice plane. Typical mesh has about 1000 parabolic brick finite elements.

The motion of a charged species in the electric field can be determined by incorporating an electrokinetic transport mechanism in the species equation. The transport of the species is through the combined effect of the electroosmotic motion of the carrier fluid and the electrophoretic transport of the species under the effect of the applied electric field.

The numerical analyses presented above are derived under the following assumptions –

- Neutral Carrier: The carrier fluid is assumed to be electroneutral everywhere, except within the double layer.
- Dilute Sample: The carrier fluid is assumed to be predominant in calculating the physical properties of the fluid.
- Uncoupled Transport: Individual *sample* species do not affect each other as to their diffusion or mobilities.
- No Chemical Reactions: The charged sample species are assumed to be fully ionized in the mixture, and do not react with each other.

The above assumptions allow the density of the mixture to be assumed constant, reducing the problem to the incompressible form. The momentum and species equations are decoupled and can be solved separately.

The modeling of electrokinetic effects is incorporated into the FlumeCAD system. FlumeCAD is an integrated design environment consisting of 3D design, modeling and simulation software tools, which enable the creation and analysis of complex microfluidic devices. Inherent in the design flow implemented in FlumeCAD is the ability to translate from a layout and process view of the device to a solid model and to continue to a 3D device model allowing simulations that characterize the various physical phenomena present in the device. The numerical solution uses a three-dimensional finite element based engine as the back-end solver for the analyses.

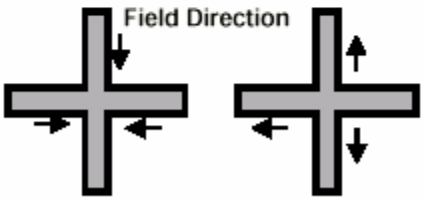

Figure 3 : Schematic of (a) Pinch and (b) Switch in intersection.

RESULTS

In this section both experimental and numerical results are presented. We begin by presenting solutions for the electrokinetically pinched flow – and the effect of the field strengths on the analyte volume in the intersection. Following that, solutions for the switched field are presented along with experimental observations for similar conditions. Finally we examine the effect of the switching potential on the width of the separated band and the residence time in the intersection – we can determine an optimal field strength for a required separation band width from this analysis.

Electrokinetic Pinch: In this section experimental and numerical results are presented for the electrokinetically pinched flow. The geometry of the intersection and the mesh used for the computation is shown in Figure 2. The geometry chosen here is similar to the experiment discussed before. The arms of the intersection are each 500 μm long. A nominal mesh contains 1000 parabolic brick finite elements – prior analyses confirmed that this resolution yielded mesh-independent solutions.

The transport mechanism in this case is electrophoretic. A schematic of the applied field that generates the pinch is shown in Figure 3. A field in the transverse channel, generating a pinch in the intersection supplements the drive potential. The species is injected from the well with the applied field and computed until steady state. The resultant species distribution is shown in Figure 4 – showing isovolumes of the species mass fraction in the intersection. The conditions chosen for the simulation are similar to experimental conditions also shown in Figure 4. The qualitative agreement shown in the figure is quite good, indicating that the simulations capture the relevant physics observed in the experiments quite well.

Effect of field strength: The volume of the species in the intersection is a function of the strength of the pinch – i.e., of the relative field strength in the arms of the intersection. As the transverse field strength, and therefore the pinch, increases, the volume decreases, since the species is confined to a smaller region within the intersection. In the switch part of the cycle, it is this volume that is will be dispensed into the separation channel. In a system, the optimal injection volume is small

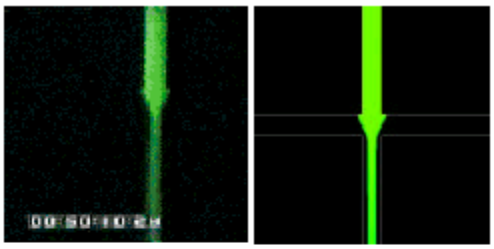

Figure 4: Electrophoretic Pinching in Cross Injector. Left Image is Experimental and Right Image is Simulation.

enough to yield a narrow band in the separation channel, yet large enough to yield an adequate signal in the detection component. In a dispensing system the injection volume is specified by that required to be dispensed. Characterization of the effect of the field on the analyte volume in the intersection is therefore an important question in the design of the injection system. In the FlumeCAD system this translates to the parametrization of the field boundary conditions over a specified range of values, with the computation repeated at each step. This variation in the boundary conditions was done through FlumeCAD's Simulation Manager, which allows the specification of a parametric variation in a boundary condition value and performs the required set of simulations and accumulates the computed data. This mechanism greatly reduced user intervention and simplified the setup and analysis of the problem.

Once the simulations are completed, the volume in the intersection is computed as a function of the field by performing a Region of Interest (ROI) integration over the intersection. The ROI defines a specific volume of the computational domain within which the contained species mass is determined. The resulting integration is shown in Figure 5 as

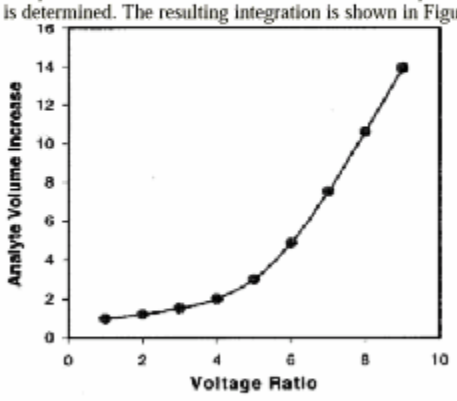

Figure 5 : Variation of Analyte Volume in Intersection with Voltage across arms of cross.

the increase in the analyte volume in the intersection as a function of the voltage ratio. The voltage ratio is defined here as the ratio of the potential difference across the fill and the pinch channel. As expected the volume in the intersection increases with increasing voltage ratio. The figure quantifies the volume in the intersection as a function of the field – the applied field required for a specific design can then be chosen from this curve.

Electrokinetic Switch: The next step in the design problem is the electrokinetic switch. The load cycle is as above, with the flow pinched in the intersection. Following the pinch, the flow is swept from the intersection into the separation channel by a field, while simultaneously current towards both top and bottom helps separate the sample plug and prevents leakage into the separation channel. A time period and a voltage and/or a current setting at each port in the design define each phase of the cycle.

Both experimental measurements and simulation results

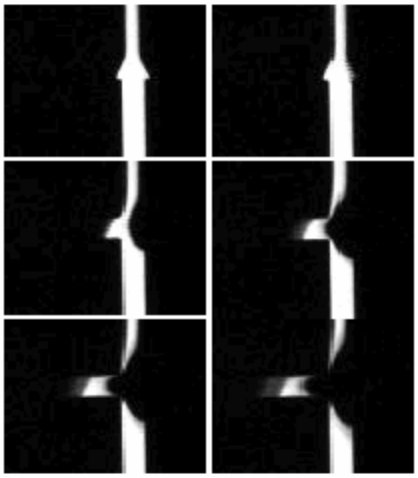

Figure 6 : Experimental Observations of Electrokinetic Switching Joint.

are presented here for electrophoretic flow. The channel geometry for the experiments were as described in the previous section. The applied current in the channel is 2 μA in the load phase with a 1μA current for the pinch, driving the species from the bottom of the image to the top as shown in experimental observations in Figure 6. The switch phase then follows with a current of 3 μA from right to left and 1 μA to pull back the species in the top and bottom channels to separate the sample plug. The time sequences shown in Figure 6 are approximately 0.1 seconds apart. Simulation results for similar conditions are presented in Figure 7 as iso-volumes of the species mass fraction, and demonstrate qualitatively good

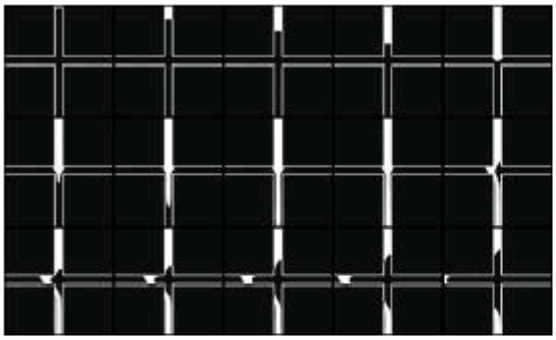

Figure 7 : Numerical Simulation of Electrokinetic flow in Switching Joint.

agreement with experiment. The shape of the pinched species as well as the shape of the plug in the separation channel is well reproduced by the simulations. This shows that the simulations appear to capture all the relevant physics in the problem and gives us reasonable confidence in the predictive capabilities of our tool.

Effect of Switching Strength: We next demonstrate the application of the simulation tools in predictive design capability by studying the effect of the field strength in the injection characteristics of the electrokinetic switch. The switching field strength affects the flow in two ways – first, in the width of the plug injected into the separation channel, and second, in the residence time of the plug in the intersection. As discussed before, the plug width is an important quality to define the injection – the residence time, on the other hand, defines the cycle time for the injection – that is, the time between subsequent injections.

The switching field is varied through the Simulation Manager, which allows granular control over the port settings in any phase in the simulation. The switching field was changed by varying the current in the separation channel from 1 to 4 μA and repeating the computation at each setting. The resulting data can be analyzed by region of interest (ROI) integrators at select locations to gain insight into the behaviour of the electrokinetic switch and to define optimal operating conditions for switch operation. Examples are shown in Figures 8-10.The band width of the dye plug in the seperation channel is shown in Figure 8 – the corresponding ROI is shown in the inset in the figure. The ROI here is analogous to an experimental point probe, such as a diode or photo-multiplier tube, positioned over the specific location to collect the flourescence of the species migrating past. It is therefore reasonably representative of conventional experimental measurements for such design problems.

The band width of the injected plug can be determined by the "broadening" of the plug through the ROI, as the change in its peak width at half maximum. The four curves in the figure correspond to differing values of the switching current. The current in the "pull-back" arms of the intersection was maintained at 1μA for all the cases. The resulting dependence of the band width as a function of current in the separation channel is extracted from the figure and presented in Figure 9. The volume of the injected band can also be computed as the integral under the curves and is also shown in the figure on the secondary axis. The band width drops as a function of increasing current, as expected. As the switching current increases further, the injected band width appears to asymptote to a minimum value. As discussed before the band width at injection is one of the qualities that characterizes injection –in general, the smaller the injected band width, the better. However, as the figure indicates, the net volume injected also drops with increasing fields. This strongly affects the homogeneity of the injected band, since species that are lighter or have greater charge are likely to be larger components of the band in comparison to heavier species or species with lesser charge – larger band widths would tend to be more homogenous. In the case of the Therefore the desirable band width, and consequently, the field, is an optimal compromise

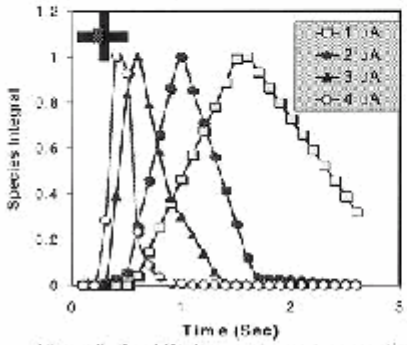

Figure 8: Band Width at entrance to separation channel as a function of switch current.

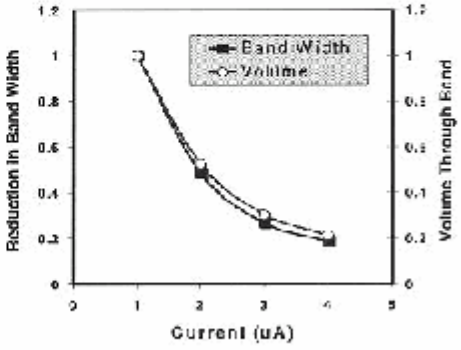

Figure 9. Reduction in Injected Band Width as a function of Field Strength for Electrokinetic Switch.

between the above two factors – curves such as Figure 9 can be used to extract the optimal design condition.

A second issue is the residence time of the species in the intersection. In several applications such as dispensing, the electrokinetic switch is used in a continuous cycle. The cycle time is then dependent on the residence time, since a new fill cycle can only begin well after the previous switch cycle is completed. An ROI integration over the intersection region yields the required residence time as shown in Figure 10, and therefore indicates an appropriate cycle time as a function of the switching field.

Curves such as those in Figures 8-10 allow the detailed characterization of the flow physics in the injection region and can therefore be employed to determine optimal injection conditions for specific applications. Extension of the analysis to more complex geometries and chemical properties is reasonably straightforward.

Conclusions

Experimental and numerical analysis of electrokinetic switching components are presented in this paper. The analyses were conducted for a typical injector, formed by the intersection of two channels. Analyses are conducted both for the steady state pinch as well as the electrokinetic switch. The numerical results show reasonably good agreement with experiment in both cases – demonstrating the capability of the design tool in capturing the relevant physics in the system. Design analyses are conducted to characterize the injection process to extract behaviourial models for the injection process to quantify the band width, volume and residence time of the injection as a function of the applied fields. The results indicate

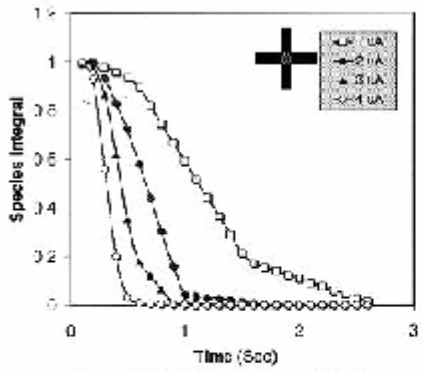

Figure 10: Residence Time of Analyte in Intersection as a function of Switching Current

that the band width in the separation channel decreases as the switching field increases – the corresponding injected volume decreases as well. The residence time of the species in the intersection also decreases with increasing field. The optimal injection for a particular system can then be extracted from such analyses. Extensions of this analysis to different injector configurations as well as different analytes is relatively straightforward.

Acknowledgements

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NOVEL DESIGNS FOR ELECTROKINETIC INJECTION IN μTAS

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Abstract

Novel designs for electrokinetic injection are presented in this paper. The designs emerge using CAD analysis of the injection process. The designs are aimed at improving the separation efficiency of electrokinetic injectors by providing a narrower and more symmetric band in the separation column in comparison to the classic injector case. Two designs, the first using a three-step switching sequence and the second using a six-port injector are presented. In both cases, the injected band shape is greatly improved. The corresponding separation efficiency is also expected to improve and has been confirmed subsequently by experiment.

Keywords: Electrokinetic Injection, CAD, Simulation, Switching.

I. Introduction

There is a wide interest in micron-scale integrated chemical/biochemical analysis or synthesis systems, also referred to as lab-on-a-chip or μTAS [1-2]. The basic operations in a typical system are sample injection, mixing, chemical reaction, separation, and detection. Systems employing electrokinetic, pressure driven and pneumatic mechanisms have been successfully demonstrated. Complicated relationships exist between the microchannel geometries, the device operating conditions, and the behavior of the multi-component fluids transported. Researchers have hitherto been forced to use costly trial and error methods to understand and design such microfluidic systems.

Computer-aided Design (CAD) tools have emerged in the past few years to assist in the design of these systems. CAD tools provide greater insight into the fundamental physics governing the behavior of these systems, and allow the exploration of a much larger parameter space in an efficient manner, in comparison to experiment. Several researchers have reported CAD-based analyses of microfluidic components [3-6]. These include components used in injection [3,4], transport [5,6], as well as mixing and reactions. These analyses were generally aimed at demonstrating numerical capability and fundamental understanding of the phenomena. In most cases, qualitative agreement with experiment or analytical results was provided to demonstrate the capabilities of the CAD analyses in adequately simulating the observed physics.

The real advantage of CAD tools, however, lies in their ability to design – that is, to create new designs or extend and optimize existing designs to make the components better. This may happen through better understanding of the component physics, or, simply, through thorough examination of the parameter space. In either case, CAD has the advantage over experimental techniques. Insertion of CAD into the design cycle can therefore reduce both the number of expensive experimental iterations and the time required for the design.

In this paper we demonstrate the capability of CAD tools to enable better design of μTAS components, by specifically focusing on one component – the electrokinetic injector. We will begin by presenting experimental and numerical results for the conventional pinched injector – to show that electrokinetic injection is well understood and predictable using CAD tools. We will then explore two mechanisms of improving the performance of the injector in delivering a sample into the separation column that is more ideally suited for separation than the conventional injector.

II. Numerical Methodology

The basic equations describing the fluid motion are the Navier-Stokes equations with appropriate electromigratory flux terms to represent the effect of the applied electric field on the carrier (electroosmosis) and/or the charged species (electrophoresis). The modeling of electrokinetic effects is incorporated into the FlumeCAD system. FlumeCAD is an integrated design environment consisting of 3D design, modeling and simulation software tools, which enable the creation and analysis of complex microfluidic devices. Inherent in the design flow implemented in FlumeCAD is the ability to characterize the behaviour of a device as a function of the various physical phenomena in the device.

The switching analyses presented here assume that the electrical field sets up instantaneously, relative to the species transport. The species is also assumed to be dilute in the buffer – i.e., it does not affect the material properties of the buffer during transport. This allows the field calculation to be decoupled from the species transport – the switching simulation is thus reduced to a sequence of electrophoretic transport simulations.

III. Classic Electrokinetic Injection

The simplest switching component is an intersection of two channels. Such intersections are surprisingly powerful tools that enable the definition of sample plugs at the picoliter level [2]; this in turn allows microfabricated electrokinetic systems to outperform their conventional counterparts by orders of magnitude [7]. The switching components are employed in separation and dispensing systems to inject the sample from the load channel to the separation channel. A typical system employing such switching components is presented in Figure 1, showing a microfluidic system fabricated by etching and bonding in glass.

The switch is operated as follows: the drive potential transporting the species into the intersection is supplemented by a field in the transverse channel that shapes a plug of a specified volume by generating a "pinch" in the field. Following the pinch, the flow is swept from the intersection into the separation channel by a field, while, simultaneously, current towards both top and bottom helps separate the sample plug and prevents leakage into the separation channel. A time period and a voltage and/or a current setting at each port in the design define each phase of the cycle.

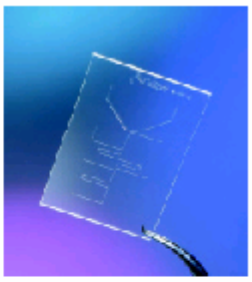

Figure 1 : Lab-On-Chip analysis system showing network of etched interconnected channels. The intersections of the channels form the injection locations.

Simulation results for the typical switch are shown in Figure 2 and compared with experimental observations in Figure 3. The results show good qualitative agreement. Greater details for both the simulation and experiment are reported in [8]. The agreement with experiment gives us confidence in the ability of the CAD tools to predict the behaviour of electrokinetic injectors. Consequently, we then focus our attention to the design of injectors that have better injection characteristics.

One of the parameters defining optimal injection is the band shape and width in the separation column. In the classic injection the band is the size of the channels, broadened by diffusion and field, and partly restrained by the "pinch" current. As shown in Figure 2 the plug is trapezoidal in shape. This broadening limits the possible resolution of the following separation column, causing the separation column to be longer than necessary. Designing injection to achieve a plug that is symmetric and narrower than the channel geometries is therefore highly desirable.

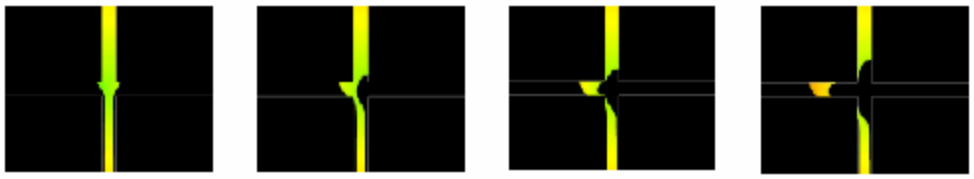

Figure 2: Simulations of electrokinetically Switched injection (the classic injector). The switching sequence has two phases (load and switch).

Figure 3: Experimental images of switched injection (the classic injector). Again there are two phases similar to Figure 2 above.

The shape of the injection plug in the intersection, and the subsequent separation, is governed by several parameters. Prominent among these is the geometry of the intersection and the switching fields applied. We have explored both these options in our attempt to design better injectors. Several designs were attempted – we will present two specific examples here – first, an alteration of the switching field sequence, and second, a geometry variation.

IV. Alternative Injector Designs

The first approach to generate a better injection plug is to insert a flow reversal between the load and the switch cycle. This allows the sample plug downstream of the intersection to be pulled back into the intersection prior to switching. The switched plug is now actually narrower than the intersection itself. The pull-back also removes the asymmetry arising due to the pinched field – the resulting plug in the separation column is both narrower and straighter than the conventional injector. The sequence of operations is shown in the simulations in Figure 4. This injection plug will yield shorter separation lengths in comparison to the conventional injector. Experiments were conducted to verify the injection sequence *after* the simulations and have verified the behaviour observed [8] in the simulations and have demonstrated significantly higher separation efficiency compared to the classic injector. The smaller separation lengths result in higher throughputs in the assays. An additional advantage is in the reduction of the field strengths required for the separation, which may have added benefits in the manufacturability of the device.

The drawback of this approach, however, is that it requires an additional electric field switching step, which needs to be controlled carefully. An alternative approach that has similar behaviour can be constructed by modification of the geometry and retaining the two-step switching pattern of the electrokinetic injectors. An example of this is the six-port injector, shown in Figure 5. This injector is made up of two intersections, one downstream of the other in the load cycle. The pinching is accomplished in a manner similar to the classic injector. As the sequence shown the pinch results in a narrow band at the second intersection. Switching at this intersection then results in the narrower band being injected into the separation column. The separation efficiency for this injector should also be significantly better than the classic injector.

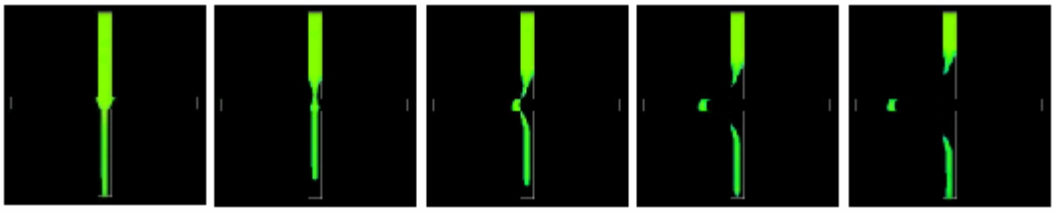

Figure 4: Reverse Injection Process showing Pullback prior to switching. The cycle is accomplished by a three-phase switch in the field – the load, pull-back and switch phases.

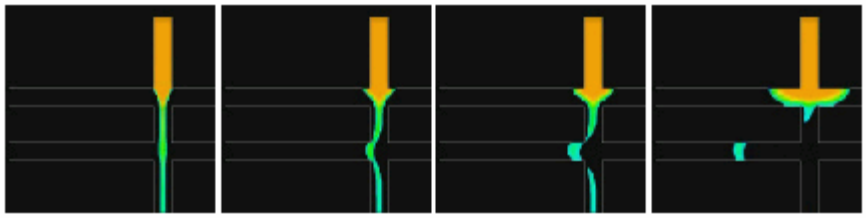

Figure 5: Six-Port injector. The cycle is two-phase – a load cycle and a switch in the downstream switch cycle.

V. Conclusions

Novel designs for electrokinetic injectors have been presented in this paper. The designs use a CAD tool that has been validated by comparing against experimental results for the conventional cross injectors. The new designs are aimed at creating a narrower and more symmetric band in the separation column. Effects due to electrical field sequences as well as geometry were considered in the designs. Specific examples demonstrating better injection band characteristics for both cases are presented here. The first case is a modification in the field using a pull-back step between the load and the switch cycle. The second case is a modification in the geometry using a six-port injector, where the switching step is actuated in the intersection downstream of the pinched intersection. In both cases the band in the separation column is narrower and straighter. The resulting separation efficiency is expected to be significantly better and has been verified by experiment discussed elsewhere.

The numerical experiments presented here demonstrate the usefulness of CAD in the design of more efficient devices and in the optimization of existing devices in μTAS.

Acknowledgments

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DESIGN ANALYSIS AND 3D MEASUREMENT OF DIFFUSIVE BROADENING IN A Y-MIXER

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Abstract:

Diffusive broadening of a low molecular weight species in pressure driven flow is studied using both experiment and numerical analysis. Confocal microscopy allows experimental visualization of the three dimensional nature of the diffusion. Numerical results support the experimental results, and are used to provide insight into design questions about devices involving diffusive mixing.

Keywords: Diffusion, CAD, Y-mixer, Confocal Microscopy

I. Introduction

The physical phenomenon of diffusive broadening has found many applications in the field of microfluidics. One of the most common is diffusive mixing of chemical or biological compounds, for the purposes of reactions or chemical sensing[1,2]. Others include the study of fast chemical reaction rates at steady state, the fabrication of microelectrodes, and the patterning of various compounds on channel walls [3]. All these applications require a detailed understanding and characterization of the transverse diffusive mixing of two miscible fluids undergoing laminar flow in microchannels.

This work presents results that demonstrate the three dimensional nature of diffusion in pressure driven flows. Experiments using a Y-mixer and a simple reaction were performed, and confocal microscopy was used to visualize the diffusive mixing in three dimensions. These results verify simple theoretical arguments for the scaling of diffusive width with transport length and flow rate. Numerical analysis was used to investigate the effects of diffusive broadening in devices using standard fluorescent microscopy detection systems.

II. Theoretical Analysis

Theoretical arguments to predict the scaling of transverse diffusive width in pressure driven flow have been made by the Harvard University group[4]; a brief summary will be given here. Using dimensional analysis, the thickness of the diffused layer in regions of uniform flow has been found to vary according to $(Dz/U_m)^{1/2}$, where D is the diffusion coefficient, z is the axial distance, and U_m is the flow speed. An extension of the Leveque problem is used to show that the diffused width in regions of shearing flow varies according to $(DHz/U_m)^{1/3}$, where H is the height of the channel.

III. Experiment

We fabricated microfluidic channels using the "rapid prototyping" technique described previously[3]. The channel structure was defined photolithographically in photoresist on a silicon wafer. Poly (dimethylsiloxane) (PDMS) pre-polymer was then cast and cured on this composite wafer / photoresist structure. A PDMS membrane with the negative relief

corresponding to the channel structure was removed from the wafer and sealed to a clean glass cover slip. A syringe pump drove the fluids into the two inlets at a constant flow rate.

We visualized the region of diffusive mixing using confocal fluorescent microscopy (Leica TCS). Fluo-3 is a commercially available, non-fluorescent compound that forms a strongly fluorescent 1:1 complex with a calcium ion (K_d = 0.39 μM). The formation of the complex is diffusion-controlled, therefore we could visualize the region of diffusive mixing by observing the concentration of this complex near the interface between flowing aqueous solutions of 5 μM fluo-3 and 1 mM $CaCl_2$ (Figure 1). At a given axial distance z from the point where the streams join, the diffusive mixing is more extensive (i.e. the fluorescent region is broader) in the slower-moving fluid near the wall of the channel than in the middle of the channel. At low flow velocities we observe some interdiffusion in the dead volume of the Y-junction (Figure 1), and we assume that its effect on the scaling behavior is negligible. There is also a pronounced asymmetry in the diffusion profile, because Ca^{2+} has a higher diffusivity (D = 1.2×10^{-9} m^2/s) than fluo-3 (D = 1.0^{-10} m^2/s) and because of the differences in concentrations of $CaCl_2$ and fluo-3.

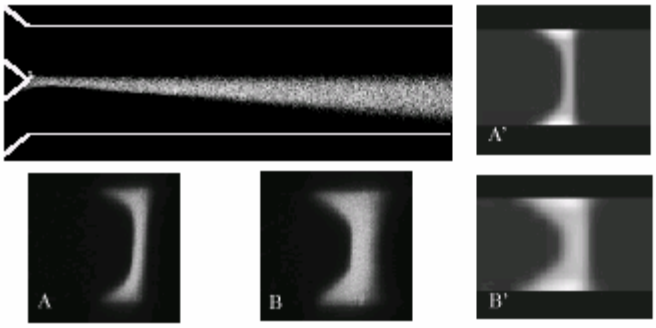

Figure 1: Experimental images from confocal microscopy (left). The corresponding simulated images (right) are qualitatively similar to the experimental images.

To test the theoretical predictions, we analyzed experimental data with Scion Image. We smoothed the 512×512 pixels images of fluorescence (such as shown in Figure 1) corresponding to 100×100 mm^2 xy scans before the analysis. For a given x (on each image we analyzed images only near x = 0 and near x = H/2) the width d(z) of the region mixed by diffusion was taken to be the width of the fluorescent region with the intensity above 0.2 of the maximum intensity. The spreading d(z) was always sufficiently small to be in a flow with uniform velocity profile in the y-direction.

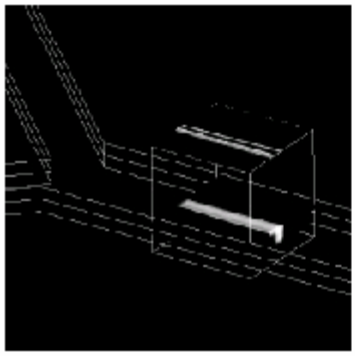

Figure 2: Standard fluorescent microscopy experiments effectively integrate in the vertical direction.

IV. Numerical Analysis

Numerical analysis can be a valuable tool for the design of microfluidic systems. Once anchored by experimental results, numerical results can predict the operation of the device over a range of parameters and geometries. Numerical analysis was performed using FlumeCAD [5]– an integrated design tool that enables the design and modeling of complex microfluidic devices. The Y-mixer was modeled by solving the incompressible Navier-Stokes equation for the velocity and pressure fields. The steady-state velocity field was then used in the coupled solution of three species transport equations – two reagents and one product. In

order to compare with the experimental results, the effective rate for the binding reaction was assumed to be infinite. The concentration of all three species was assumed to be dilute, so that the properties of the carrier were constant. The above equations were solved using a fully three-dimensional finite element based CFD engine.

Many experiments are performed using standard fluorescent microscopy techniques, which have the effect of integrating the three dimensional fluorescent signal in the vertical direction (as in figure 2). This obscures the effect of the three dimensional diffusion profile. Using numerical integration, the effective diffusive widths that would be seen with standard microscopy techniques were calculated.

V. Results

Confocal microscopy was used to measure the diffusive width at a sequence of locations in the channel, for a maximum flow rate of 16 cm/s. Results shown in figure 3 agree well with theoretical predictions. In the center of the channel, where the flow is uniform, the width scales as the 1/2 power of the distance down the channel. Near the wall, the scaling behaves as the 1/3 power of distance. Experiments were also performed at several flow rates, and the results are shown in figure 4. The diffusive width scales as the −1/2 power of flow rate in the center of the channel, and as the −1/3 power of flow rate near the channel wall, which is in agreement with theoretical predictions.

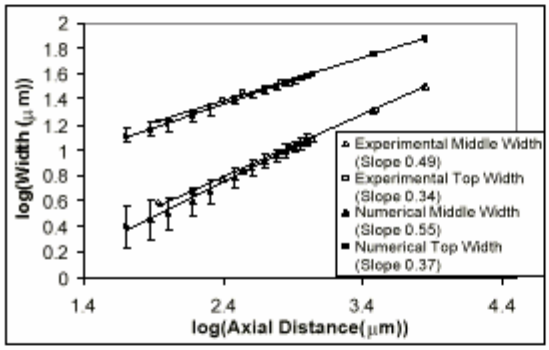

Figure 3: Experimental and numerical results for average flow velocity 8 cm/s.

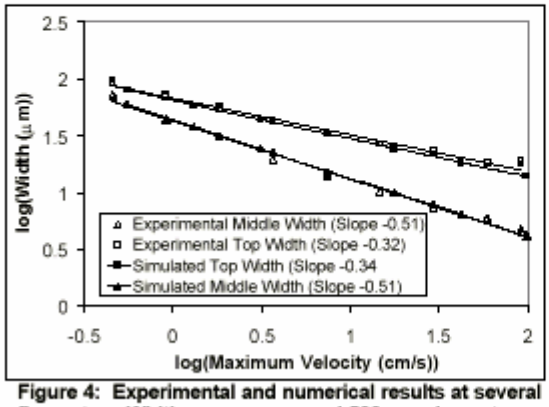

Figure 4: Experimental and numerical results at several flow rates. Widths were measured 500 mm downstream from the intersection.

Numerical simulations agree well with the experimental results. The distribution of the fluorescent compound at two positions in the channel compares qualitatively with the experimental results (Fig. 1), and the simulations also predict the same scaling laws for diffusive width as a function of axial distance and flow rate (Figs. 3,4).

Vertical integration of the three-dimensional simulated results, to mimic a standard microscopy setup, gives some interesting results (see figure 5). The scaling of the diffusive widths with distance depends on the threshold used. With a lower threshold (20%), the width scales roughly as the 1/3 power of distance. However, as the threshold is raised toward 80%, the scaling law approaches the 1/2 power of distance. This interesting result can be explained by figure 6. The layer near the wall, where the 1/3 power scaling takes place, is thin for the flow regimes investigated here (this can be visualized from experimental and numerical images, figure 1). A line plot of intensity across the

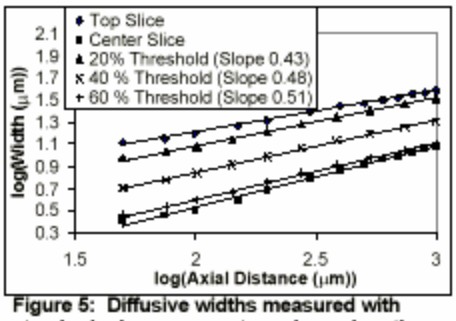

Figure 5: Diffusive widths measured with standard microscopy setups depend on the threshold used.

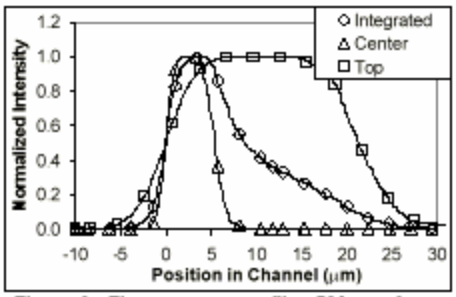

Figure 6: Fluorescence profiles 500 mm from the intersection. The shape of the integrated peak explains the effects of the different thresholds.

channel shows that this results in a wide base on the peak shape (figure 6); so a lower threshold effectively gives the width in the shear layer. As the threshold is raised, the total amount of fluorescence in the shear layer drops below the threshold, so the 1/2 power scaling from the center of the channel is recovered.

VI. Conclusions

Both experimental and numerical results agree well with theoretical predictions for the behavior of diffusive layers in pressure driven flow. The results demonstrate that three-dimensional effects can be important for the operation of devices using this type of diffusion. If uniform velocity diffusion scaling laws are applied blindly, device performance may not be as expected.

Numerical results have provided some additional insight that may help to design laminar flow mixing devices more accurately. When using a standard confocal microscopy detection system, the use of a high threshold for peak width calculation can ensure that the desired width scaling with distance is achieved.

Acknowledgments

This work was funded by the DARPA Composite CAD program, under FlumeCAD (Grant no. F30602-98-2-0151) and NetFlow (Grant no. F30602-96-2-0306).

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Design Analysis of No-Moving-Parts Valves for Micropumps

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ABSTRACT

A design methodology for extracting component models for fluid dynamic devices is presented. The analysis uses Memcad's suite of design tools to build the solid model and perform the analysis and post-analysis to extract the parametric variations of interest. In this paper, we demonstrate this capability by analyzing two types of no-moving-parts (NMP) valves used in micropumps: the diffuser type and the Tesla-type valves. The results indicate that the Tesla-type NMP valve has a higher pumping efficiency, and therefore a higher throughput, for the same Reynolds number flow, compared to the diffuser type valve. The parametric behavior reported by Memcad can then be used to generate a reduced-order model for system level simulations in a straightforward manner.

INTRODUCTION

There is considerable interest in recent years in the development of micropumps as components in microfluidic systems (van Kuijk (1997) for a review). These pumps have applications in a wide variety of areas such as chemical, biomedical and electronic cooling, among others. Micropumps have two basic forms of valves: with and without moving parts (Forster et. al., 1995, Gerlach and Wurmus, 1995, Olsson et.al., 1995). Pumps with valves having moving parts have many drawbacks at the microscale. Wear and fatigue of the moving components can cause reduction in performance and reliability. They are not conducive to handling multiphase fluids because of potential clogging. Pumps with valves without moving parts have significant advantages because of their simplicity, ease of manufacture and ability to transport multiphase fluids. These pumps consist of a fluid cavity and two valves, with an oscillating pressure gradient applied across them. Their principle of operation is based on the rectification of the fluid by the valves. For the same pressure drop, the flow in the forward direction through these valves is greater than the flow in the reverse direction. In a continuous cycle, therefore, there is a net transport from the input to the output port of the pump. The difference in the flow rate in the forward and reverse direction is dependent on the relative magnitude of rotational and/or convergent flow phenomena in the valves in one direction compared to the other. Good designs generally aim at maximizing this difference.

An appropriate design methodology for these pumps is through a system model that is based on independent models for each of the device components. The pumps have a resonance frequency that is dependent, among other things, on the mass of the fluid in the valves. The design of the valves is therefore critical to the efficient operation of these pumps. Design considerations also include the efficiency of the valves, defined as the ratio of the net flow rate through the valve to the average flow rate, and the resistance to flow in the valves. Additional considerations include the frequency and amplitude of pump operation. A good design for these valves is an optimal compromise between the diodicity and the flow resistance.

System models of pumps with NMP valves were developed by Olsson et. al. (1995) and in a more detailed manner in Bardell et. al. (1997). These models use component models derived theoretically and validated by comparison with experiment. Accurate component models are essential to the development of a system model that adequately characterizes the behavior of the system. Individual component models are, however, hard to extract experimentally in a complete pump. Numerical methods can however be used for this purpose and are the focus of this paper. We present here, a framework to develop a component model for the NMP valves using the capabilities of the Memcad system.

Pumps with NMP valves have hitherto been designed using the diffuser-type valves. (Gerlach and Wurmus, 1995, Olsson et.al., 1995). A second design that has been implemented uses the Tesla type valves shown in Fig. 1. Details of the design are discussed in Forster et. al (1995). A system model based on individual models for the valve and chamber components was developed using an analytical valve resistance model based on the assumption of laminar flow. A more accurate representation might be a full numerical solution of the flow to extract the valve resistance. In this

paper, we demonstrate the capability of the Memcad software for that purpose.

We simulate and analyze both the Tesla-type and the diffuser-type NMP valves and compare the relative performance of the two.

NUMERICAL SETUP

The NMP valves chosen here were analyzed using Microcosm Technologies' Memcad software tool. This tool comprises of a layout and process design phase, automatic construction of solid models and a suite of multi-domain and coupled domain solvers for a wide range of MEMS and microfluidics problems. A higher layer of simulation management enables the extraction of component models by simplifying the specification of parametric variations of interest.

The fluid dynamic problem was solved using a fully three-dimensional finite-element based solver for the Navier-Stokes equations. Three-dimensionality cannot be ignored in these problems since the ratio of surface area (causing the pressure drop) to the volume (the flowrate) is significant. Even at high flow rates the Reynolds number is relatively small – on the order of 200-400 – because of the small dimensions of the micro-valves. The flow is therefore laminar. Issues of mesh refinement were resolved by requiring nominally at least ten nodes within the boundary layer. Mesh independence studies were conducted to verify this constraint and are discussed briefly below.

MODEL CONSTRUCTION

The setup for the analysis began by constructing a layout for the device under consideration. In this case the layout used in the pump designs were available in CIF/GDS format. The process used for the fabrication was then specified in the process editor. Using Memcad's Membuilder (Osterberg et. al, 1995) module, a solid model was constructed automatically from the mask and process definition in I-DEAS. The solid model constructed for the T45 section is shown in Fig. 1. The constructed model was then meshed using parabolic brick elements. Flow symmetry was assumed in the depth plane in the Tesla-type valves and in the depth and transverse plane in the diffuser valves. This assumption greatly reduced the number of elements required and made the computation tractable on a conventional workstation.

RESULTS

In this section results for both types of valves are presented. We will begin with a brief discussion of mesh refinement issues. The Tesla-type valve is discussed next including validation with experimental measurements. Finally, results for the diffuser valve are presented and compared with experiment and with the Tesla-type valves.

Mesh Refinement : In any numerical analysis the ability of the discretized mesh to accurately represent all the fluid physics is critical to accurate solution of the problem. In this analysis the performance of the valve was obtained by computing the flow rate induced by an applied pressure differential across the valve. The induced flow was a function of fluid resistance due to the valve walls, and losses in regions of separated-flow. Inadequate resolution of the flow will underestimate losses and predict incorrect results.

In our analysis the independence of the predictions from the mesh resolution was analyzed by successively refining the mesh and computing the flow for one pressure drop. The computed flow rate was then plotted against the mesh size and shown in Fig 2 for a pressure drop of 0.1 atm. – an appropriate resolution was then extracted from this curve at the convergence of the computed flow rate.

Computations were performed at average element size of 5, 10 and 22 microns in the transverse direction (along with the two-dimensional case). This corresponds to 22, 11 and 5 parabolic elements across the valve (the valve inlet port width is 114 microns). As the figure shows there was a considerable difference between the 22 micron and the 10 micron case. The difference between the 10 micron and 5 micron case, was however, almost negligible. For this reason, we chose the 10 micron case as the baseline for the calculations. Note that the mesh was highly stretched in the transverse direction (from centerline to wall) – therefore the element thickness in the region near the wall is considerably less than the average.

Tesla-type valve : The T45 valve is similar to the T45-R valve (Forster et. al, 1995), except that it has a single loop as shown in Fig. 3. Each channel is 114 μm wide with a 120 μm etch depth. As discussed before, the efficiency of the valves is largely dependent on the difference in the flow phenomena in the forward and reverse direction. The presence of rotationality and reattachment in the flow increases this difference and, thus, the valve efficiency. The loop is geometrically designed for this purpose.

The mesh used in the simulations is shown in Fig. 3. As in the diffuser case, the simulations took advantage of flow symmetry in the depth direction (normal into the plane of Figure 3). As before, every alternate element is shown in the figure for clarity. The mesh used approximately 3050 parabolic brick finite elements. The problem was set up by applying normal stress boundary conditions on the inlet and exit (assuming fully-developed flow at the inlet), and applying the requisite no-slip and symmetry constraints on the boundaries. The flow rate was then computed from the results of the simulation. To generate the required resistance curve of pressure versus flowrate, the applied normal stress was varied over a specified range. This variation in the boundary conditions was done through Memcad's Simulation Manager, which allows the specification of a parametric variation in a boundary condition value and extracts the required curves of interest. This mechanism greatly reduced user intervention and simplified the setup and analysis of the problem.

Each simulation required approximately 4 hours of CPU time on a workstation (HP C160) for convergence. The results from the computations are shown in Figs 4-7. Fig 4 shows the pressure field over a slice plane through the center of the valve parallel to the plane of the flow for a pressure drop of 0.2 atm. Both the forward and reverse directions are shown in the figure. In the forward direction the pressure drop was relatively gradual over the core region of the valve. The pressure drop in the reverse direction, on the other hand, indicated the presence of a stagnation region at the intersection of the two arms of the valve. The incoming flow separated around this stagnation point and converged later near the exit plane. This geometrically induced rotation and subsequent convergence of the flow was dramatically different from the flow pattern in the forward direction. This was even more evident in the velocity vector field for the two cases, shown in Fig. 5. In the forward direction, the flow barely sensed the presence of the "bleed" path – and was driven entirely through the straight leg of the valve. In the reverse direction, on the other hand, the flow separated into

the two legs and reconverged at the downstream intersection. The increase in the travel path of the flow and the momentum interaction at the convergence of the two paths resulted in a greater pressure drop. This causes an increase in the diodicity and thus in the efficiency of the valve.

The flow rate induced by the differential pressure is shown in the graph in Fig. 6 over a range of pressure drops. The experimental measurements are also shown in the figure. The simulations showed reasonable agreement with experiment over the range of pressure drops simulated. The net flow rate generated from the valve, defined as the difference in the flow rate in the forward and reverse direction for the same pressure drop, is shown in Fig. 7 as a function of the applied pressure. The efficiency of the valve, defined as the net flow rate divided by the average flow rate is shown in Fig. 8. In both cases, experimental data is also shown. The simulations tend to underpredict the net flow rate slightly – the agreement however is reasonably satisfactory, and the behavior of the device was accurately captured. These curves, in Figs. 6-8, essentially represent the component model for the valve that can then be used in the system model. It is important to note here that these curves, and eventually the system model representation of the valve, were obtained from a single Memcad run without intermediate user intervention.

Diffuser-type Valve : The D3 valve used in this analysis has a 60 μm etch depth, a 114 μm wide throat, a diffuser section 1101 μm long and 322 μm wide, and a nozzle section 419 μm long and 792 μm wide. The mesh used in the analysis is shown in Fig 9. Every second finite element is shown for clarity. The mesh had a total of 2880 parabolic brick elements. Computation times in the diffuser valve case were comparable to the T45 case discussed above.

The pressure field for one representative computation corresponding to a pressure drop of 0.2 atm is shown in Fig. 9. In the forward direction the pressure drop was relatively gradual through the diffuser region. In the reverse direction the drop was much more rapid, as expected for nozzle flow. The effect of the asymmetry is seen in Fig. 10 showing the pressure versus flow rate curves over a range of applied pressures. Experimental data is also plotted on this graph (symbols) showing reasonable agreement between experiment and simulation for both the diffuser and the nozzle direction. The geometrical asymmetry was manifested in the presence of recirculation regions in the flow in the nozzle direction. The recirculation region essentially decreased the available flow area locally, leading to a higher overall pressure drop and a decreased flow rate. In the diffuser direction, on the other hand, the flow remained smooth. The net effect of the asymmetry was the difference in the flow rate in the forward and the reverse direction, which, as discussed before, provides the pumping effect.

Comparison between valves : The available results for the Tesla-type and the D3 valve allow us to compare their performance in the configurations that were tested. As discussed before, the difference in the flow rate in the forward and reverse direction, and therefore the valve efficiency, is dependent on the relative magnitude of rotational and/or convergent flow phenomena in the valves in one direction compared to the other. The Tesla-type valve is geometrically designed to increase these effects and therefore would be expected to have a greater net flow rate and efficiency for the same applied pressure drop. Figures 11 and 12 compare the flow rate induced and the efficiency of the valves respectively. As the figures show, in the current configuration, the Tesla-type valve generates a larger flow rate than the D3 valve, and at a higher efficiency.

Using curves such as Figs 11-12 as an anchor, we can now implement Memcad in the inverse design problem – i.e., to determine the optimal configuration for the highest efficiency in the valves studied.

CONCLUSIONS

Micropumps with NMP valves are a promising new development in the microfluidics field. They have several advantages over conventional pumps in terms of reliability and reduced wear. The design of these micropumps is strongly dependent on the diodicity and the characteristics of the actuation membrane that drives the pump and the fluid mass through the pump. A good design analysis of such a device is dependent on a good system model, which, in turn is dependent on good component models. Individual component models are hard to extract from experimental analyses, but can be extracted from numerical simulations. These simulations need to be anchored with experimental data for validation.

In this paper we have demonstrated the capability of the Memcad software in the design analysis of devices of this nature. Starting with the layout and a process definition, the solid model can be automatically generated within Memcad and analyzed with an available suite of solvers and a higher level of simulation management to extract parametric curves of interest. We have applied this capability to the analysis of a Tesla-type valve and a diffuser-type valve to extract the efficiency of these valves over a specified pressure range. The results indicate that the T45 valve is considerably more efficient than the D3 diffuser valve.

An important aspect of the simulations presented here, that is not easy to describe, is the ease of problem setup, analysis and post-analysis that is made possible by the design tools available through Memcad.

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Osterberg, P. M., and Senturia, S.D., "MemBuilder: An automated 3D solid model construction program for microelectromechanical structures," *Transducers 1995*.

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Fig 1 : Solid Model generated by Membuilder for Tesla T45 valve.

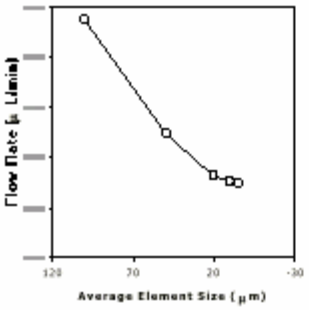

Fig 2 : Mesh Dependence study for T45 valve. Average element size is for a cube of specified size over domain.

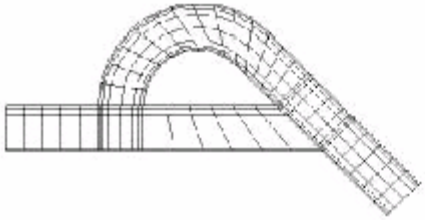

Fig 3 : Mesh used in the T45 valve calculation. Every alternate element is shown. Mesh corresponds to approximately 3050 parabolic brick elements.

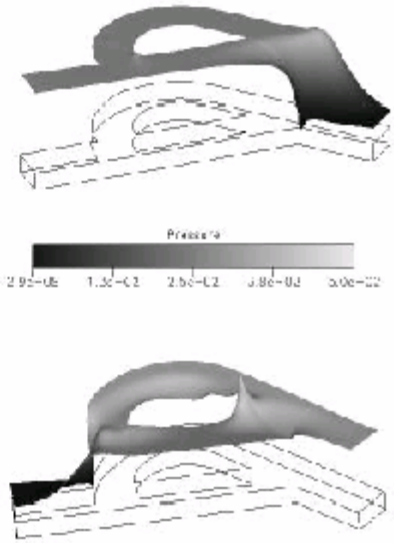

Fig 4 : Pressure on a slice plane through center of valve element. Upper figure is for forward direction flow. Units of pressure are MPa.

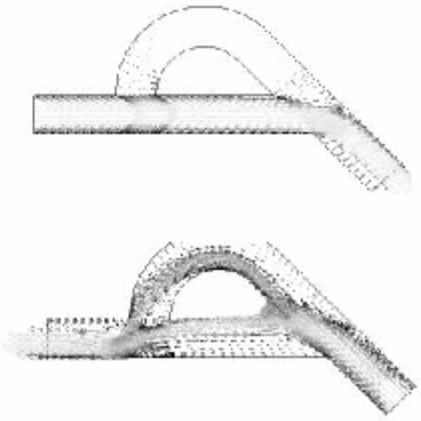

Fig 5 : Velocity Vector field on a slice plane for flow through the T45 valve element. Specified pressure drop is 0.2 atmospheres.

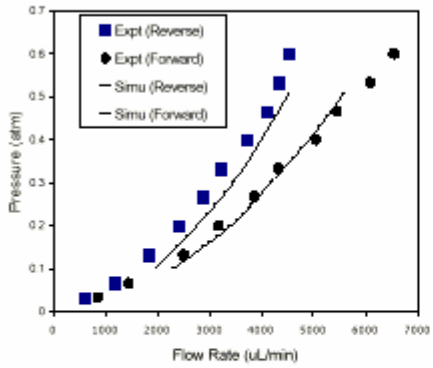

Fig 6 : Pressure vs flow rate in forward and reverse direction for T45 valve and comparison with experiment.

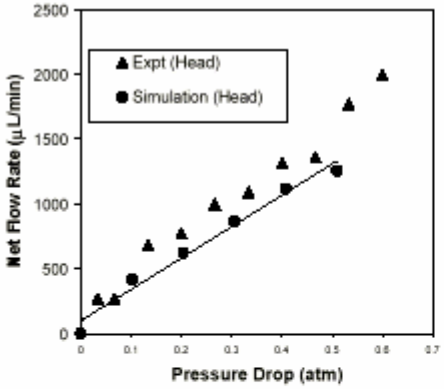

Fig 7 : Net Flow Rate in Tesla-type valve (difference in forward and reverse flow rates) vs. pressure drop. Comparison between experiment and simulation

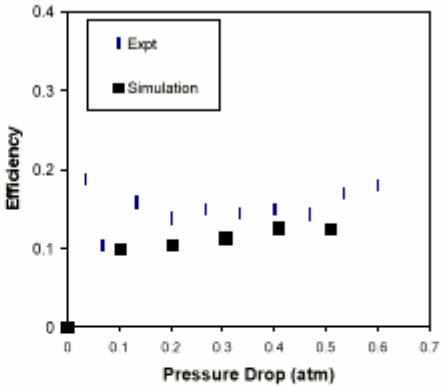

Fig. 8 : Efficiency of Tesla-type valve (ratio of net to average flow rate) vs. pressure drop. Comparison between experiment and simulation

Fig 8 : Mesh used in diffuser computations. The three-dimensional mesh has approximately 2880 parabolic elements.

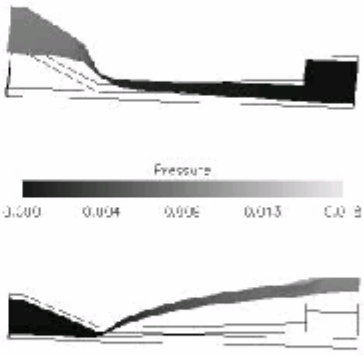

Fig 9 : Pressure field on a slice plane through center of diffuser element section. The upper figure is in the diffuser direction and the lower one in the nozzle direction.

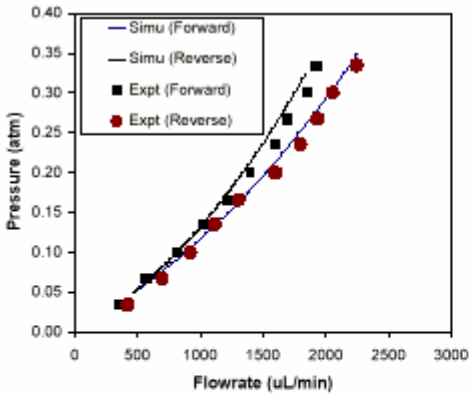

Fig 10 : Pressure vs flow rate in forward and reverse direction for the D3 valve and comparison with experiment.

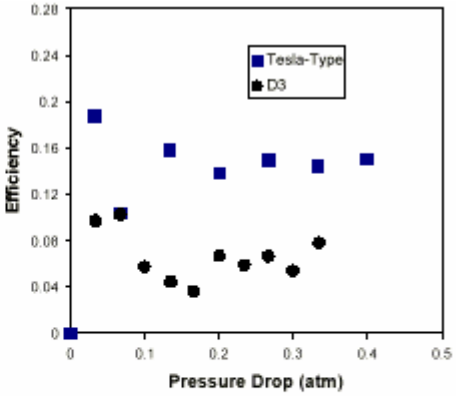

Figure 12: Comparison of efficiencies of Tesla-type and D3 valves with pressure drop. Efficiency is defined as the ratio of net flow rate (difference between forward and reverse directions) and average flow rate.

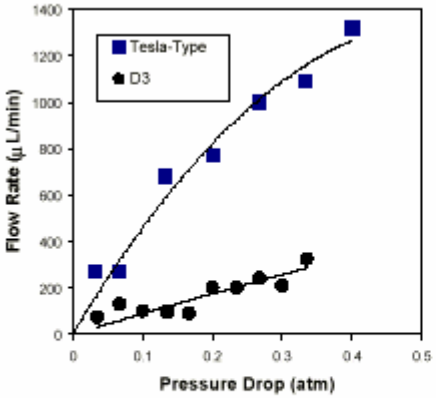

Figure 11: Comparison of net flow rate (difference between forward and reverse directions) between Tesla-type and D3 valves with pressure drop.

PREDICTIVE DESIGN OF REVERSE INJECTION MECHANISM FOR ELECTROKINETIC DNA SAMPLE INJECTION

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ABSTRACT

A novel injector designed by CAD analyses is presented in this paper. The injection mechanism uses a pull-back inserted between the pinch and the switch stages of the typical cross injector to create a band that is more symmetric and narrower than the typical injector. The resulting separation efficiency is greatly enhanced as a result of the more optimal band shape. The injector was designed using a validated CAD tool, and verified subsequently by experiments. The resulting separation efficiency achieved was significantly greater than current injectors.

INTRODUCTION

Electrokinetic microfluidic microsystems are powerful analytical tools for many applications, such as nucleic acid analysis, enzyme assays, and immunoassays [1-4]. Such systems have gained considerable importance as components in micron-scale integrated chemical/biochemical analysis or synthesis systems, also referred to as lab-on-a-chip. The basic "unit process" operations in these systems are sample injection, mixing, chemical reaction or modification, separation, and detection. Assembling a system of many "unit process" nodes requires one or more transport mechanisms to move sample and reagents through the "wires" of the system. Many of these systems rely on electrokinetic physics as their transport mechanism, although pressure and pneumatic applications have also been demonstrated. Complicated relationships exist between the microchannel geometries, the conditions under which the devices operate, and the behavior of the multi-component fluids transported in these channels. In the past researchers have been forced to use costly trial and error methods to understand and design such microfluidic systems.

CAD tools can be a valuable aid in the design of microfluidic systems. Numerical analyses provide significant insight into the fluid mechanics in these systems. They allow the extraction of material and flow properties that are generally not well documented, or that vary from application to application or from one manufacturing technology to another. Furthermore such tools help the designer to explore a much larger space of designs than is easily available from experiment, and do so in a quantitative way that enables the extraction of key parameters for improved or optimal operation of common microchemical system components.

Simulations of electrokinetic flows have been reported in the literature for both electrophoretic [5,6] and electroosmotic [7,8] flows. In [6] and [8], simulations of pinched injection have been reported in channel intersections, demonstrating the application of electrical fields to position the species plug in the intersection, prior to switching. These analyses are 2D steady-state analyses with fixed field boundary conditions. Three-dimensional simulations of pinched injection have also been reported by these authors in previous work [9]. In all these cases, the analyses were aimed at demonstrating numerical capabilities and an understanding of the fundamental physics prevalent in the device. Agreement with experiment reported in these analyses is generally good.

The capabilities of CAD tools can only be fully realized when they are applied in predictive design of a device that improves or optimizes its performance. In this paper, we present the predictive use of simulation to design an improved injector, followed by experimental confirmation of that design and the use of the improved injector to achieve the fastest separations of DNA oligos currently achievable.

Microfluidic networks have a distinct advantage over conventional electrophoresis system in the area of rapid separations. Microfluidic systems have demonstrated separations in the order of seconds in comparison to several minutes in conventional systems [3,4]. A critical parameter in achieving rapid separations is the ability to inject a narrow plug into the separation column. Typically, microfluidic system achieve this by using pinched injection in a cross injection, as shown in Figure 2. The drive potential is supplemented

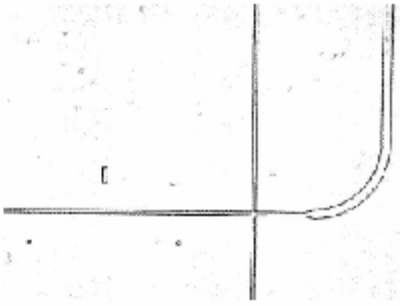

***Figure 1**. Photograph of a NS95 microchip used for the reverse injection experiments.*

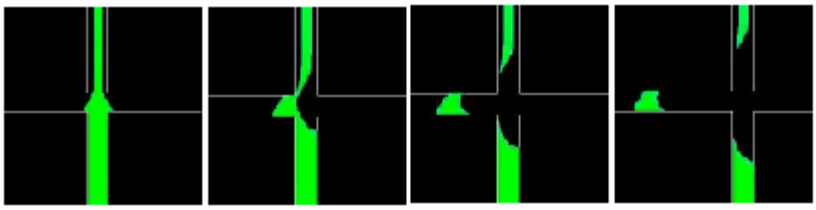

Figure 2. *Typical Electrokinetic injection process showing the pinching and the switching process.*

by fields in the transverse channels to shape the plug in the intersection prior to switching into the separation column as seen in the figure. The plug thus injected can be of the order of the channel dimension or smaller. As shown in Figure 2 the plug is broadened in a trapezoidal shape. This broadening limits the possible resolution of the following separation column, causing the separation column to be longer than necessary. Designing injection to achieve a plug that is symmetric and narrower than the channel geometries is highly desirable.

Here, we will use CAD to focus on this aspect of the injection in an attempt to improve it. We will begin with a short description of the numerical tools followed by details of the simulation. Following that we will present experimental results that corroborate our findings, resulting in an improved injector, that demonstrates faster separations at lower voltages than conventional injectors.

NUMERICAL FORMULATION

The basic equations describing the fluid motion are the Navier-Stokes equations with appropriate electromigratory flux terms to represent the effect of the applied electric field on the charged species. The basis for electrophoresis is the differential migration of the charged species ions relative to the carrier molecules under the application of the external field. The differential migration is primarily an effect of the difference in the net charge between the solvent and solute ions, although frictional effects may also have some relevance. The migration velocity of the charged species can be expressed in terms of the applied field strength as $V_{ep} = \mu_{ep} E$, where μ_{ep} is the electrophoretic mobility of the ion in the carrier species. It is important to note that in most cases the carrier does not move under electrophoresis.

The motion of a charged species in the electric field can be determined by incorporating an electrokinetic transport mechanism in the species equation. The transport of the species is through the combined effect of the electroosmotic motion of the carrier fluid and the electrophoretic transport of the species under the effect of the applied electric field.

The numerical analyses presented above are derived under the following assumptions –

- Neutral Carrier: The carrier fluid is assumed to be electroneutral everywhere, except within the double layer.
- Dilute Sample: The carrier fluid is assumed to be predominant in calculating the physical properties of the fluid.
- Uncoupled Transport: Individual *sample* species do not affect each other as to their diffusion or mobilities.
- No Chemical Reactions: The charged sample species are assumed to be fully ionized in the mixture, and do not react with each other.

The above assumptions allow the density of the mixture to be assumed constant, reducing the problem to the incompressible form. The momentum and species equations are decoupled and can be solved separately.

The modeling of electrokinetic effects is incorporated into the FlumeCAD system. FlumeCAD is an integrated design environment consisting of 3D design, modeling and simulation software tools, which enable the creation and analysis of complex microfluidic devices. Inherent in the design flow implemented in FlumeCAD is the ability to translate from a layout and process view of the device to a solid model and to continue to a 3D device model allowing simulations that characterize the various physical phenomena present in the device. The numerical solution uses a three-dimensional finite element based engine as the back-end solver for the analyses.

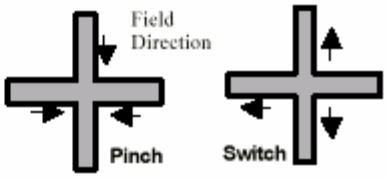

Figure 3. *Schematic of the typical two phase injection*

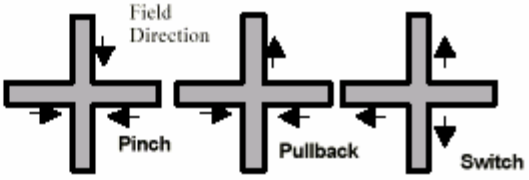

Figure 4. *Schematic of Reverse Injection including pull-back.*

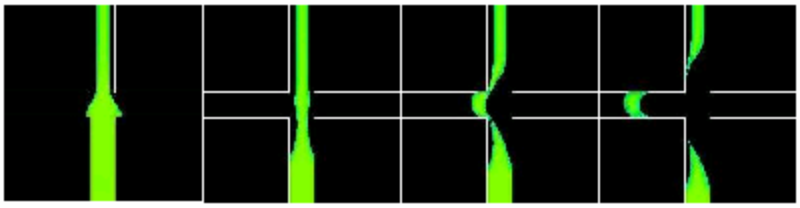

Figure 4. *Reverse Injection process showing pull-back and subsequent switching into separation column.*

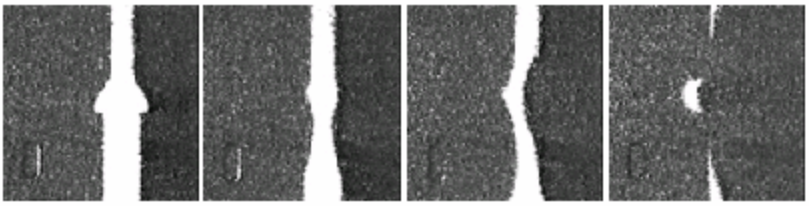

Figure 5. *Experimental verification of reverse injection predicted by numerical simulations above.*

Design Analysis

The design analyses were conducted on a cross injector. The numerical tools were first validated by comparing against experiment for the classic two-phase pinched injection. A schematic of this injection mechanism is shown in Figure 3 – corresponding simulation results are shown in Figure 2. The injection consists of a "pinch" – fields in the transverse channels supplementing the drive current – followed by a "switch" – sweeping the sample into the separation column along with current towards both top and bottom to separate the sample plug and prevent leakage. The simulations presented here were compared against corresponding experimental observations in [9] and show good qualitative agreement, indicating that the simulation tools capture all the relevant physics in the problem quite well.

As Figure 2 shows the switched plug in the separation column is trapezoidal in shape. The shape in the separation column is a consequence of the shape of the pinch in the intersection between the two channels. Since the sample is positioned in the intersection by a pinch, the shape in the intersection is trapezoidal, with the base of the trapezoid being wider than the characteristic dimension of the intersection. As the trapezoidal bands move downstream the individual fragments separate out based on their electrophoretic mobilities, and broaden based on their diffusivities. The effective band width in the separation column is determined by the width of the trapezoid base, which limits the separation efficiency.

A better injection mechanism is required to create a better sample plug in the intersection prior to separation. This can be achieved by alterations in the geometry or in the switching field sequence. One such example, showing a six-port switch, where the pinch and switch are carried out in different intersections, was presented in [10] and results in a narrower band in the separation column. A second approach termed "reverse injection", presented here, uses a three-phase switching sequence. The schematic of this sequence is shown in Figure 4. A "pull-back" phase is added between the pinch and the switch. In the creating of the pinch, the sample is positioned in the intersection by the pinching fields. Downstream of the intersection the band is significantly narrower than the width of the intersection, and is dependent on the strength of the pinching field. Adding a pull-back phase momentarily reverses the field in the drive channel, while maintaining the pinching fields as seen in the schematic. The pull-back causes the downstream band to retract into the separation column creating a significantly narrower band at the entrance of the separation column. Additionally the downstream band is also symmetric since it is not modified by the effect of the pinch. The usual switching step then follows to drive the sample into the separation column.

Simulations showing the effect of the "pull-back" are presented in Figure 5. The effect on the band width and shape in the separation column is dramatic – the band is now both narrower and straighter than the conventional injector case in Figure 2. The results indicate that we can achieve DNA bands that are symmetric and narrower than the underlying channel geometry – consequently the resulting separation efficiency is expected to improve significantly as a result of the band shape.

Experimental Verification

Following the CAD analysis, experiments were conducted to verify the predictions presented in the previous section. The separations were carried out in soda-lime glass chips with channels 10 μm deep and 30 μm wide, filled with a 6% polyacrylamide-based separation matrix. The buffer was 100 mM TAPS-Tris. For imaging

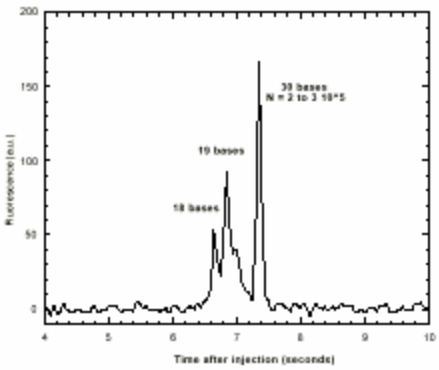

Figure 6. *Ultra-high speed separations using reverse injection process.*

studies, the samples were single-stranded DNA oligonucleotides at a concentration of 20 μM, fluorescently labeled at fluorescein wavelengths. Images were recorded on a Hammamatsu intensified CCD camera. For separations, similar oligonucleotides were used, but labeled at red wavelengths with Cy-5 dye, and at a concentration of 100 nM. Detection was carried out using a red diode laser, on a fluorescent microscope system as described earlier [3]. Experimental images corresponding to the reverse injection case are shown in Figure 6. The experimental results agree very well with the numerical predictions from Figure 5. The details of the sample behaviour including the shape in the intersection prior to switching, and the shape of the subsequently injected band, are correctly captured by the simulations. Separations from this injector are presented in Figure 6. The narrow band created by reverse injection enabled the demonstration of 7 second DNA separations in a 0.5cm long on-chip column, using only 150V (300V/cm). These are the fastest separations accomplished to date and are a result of the improved injector design emerging out of the CAD analyses.

Conclusions

The application of CAD in the design of microfluidic chip components is demonstrated in this paper, using the cross injector. In typical separations, the efficiency is limited by the width of the band in the separation column, which in turn is limited by the width of the band positioned in the intersection. Using a validated CAD tool, we have improved the injection characteristics by inserting a pull-back between the punch and the switch. This injection, called "reverse injection" retracts the narrower and symmetric band downstream of the intersection back into the intersection, and subsequently into the separation column. The injection characteristics have been verified by experiment and have yielded faster separations using lower fields than have been accomplished hitherto.

The primary conclusion of this work is the successful application of CAD to predict and improve the performance of microfluidic components. CAD also has the advantage of being able to explore a much wider parameter space to design these improved components, and hence should serve as an important component of the design process.

Acknowledgements

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Development of a Reduced-Order Methodology in the Design of Microfluidic Systems

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Abstract

This paper presents current research in the development of tools to enable the design of microfluidic systems. The design tools use detailed analyses of the physical phenomena in these devices to understand the behaviour of the specific component and extract a model representing this behaviour. The models for the individual components can then be combined in a system model for the device incorporating the interaction between the components and enabling design analyses of the entire device. Specific examples will be presented to demonstrate this capability.

Introduction

There is a wide interest in micron-scale integrated microfluidic systems for use in several applications such as sensors (flowrate, pressure or shear stress), actuators (micropumps, switches) and complete fluid processing systems (lab-on-a-chip, reactors). These systems are generally integrated systems consisting of flow components, chemistry components as well as detection/sensing components. The components span a wide-range of physical disciplines that adds to the complexity of their design. Often designers from diverse backgrounds and physical domains are required to work together and share information about the device.

Computer-aided Design (CAD) tools have emerged in the past few years to assist in the design of these systems. CAD-based analyses of microfluidic components have been reported by several researchers. [1-3]. CAD tools can be a valuable aid in the design of microfluidic systems. Numerical analyses provide significant insight into the fluid mechanics in these systems. They allow the extraction of material and flow properties that are generally not well documented, or that vary from application to application or from one manufacturing technology to another. Furthermore such tools help the designer to explore a much larger space of designs than is easily available from experiment, and do so in a quantitative way. CAD tools also assist in the extraction of a reduced-order model that describes the behaviour of a particular component, and its dependence on key parameters. Models for individual components can be coupled together to analyze and often optimize the entire microfluidic device.

Microfluidic devices generally represent the active component of a larger system. Such systems have some common layers to their design. These include the design of the actual device (design a manufacturable component), package design (design a practical package), and system design (design and improve the system or instrument the device fits into). A successful system requires the design criteria for each of the individual domains to be met successfully in an economic and manufacturable manner.

In the MEMS and IC domains the system development is enabled by the availability of design aids, which assist in the integration of all the domains of the design. These design aids provide a top-down approach to system design, which allows the designers to understand the components in the system and the effects of one component on another. In microfluidics, such aids are scarce – this greatly hampers the development of these systems. A good design tool therefore has considerable value in assisting the rapid transfer from a concept to a viable product.

In this paper, we explore the development of a design methodology for microfluidic systems. This methodology allows both the detailed analysis of the components in the system as well as of the behaviour of the system as a whole. The underlying physics in the individual components will be discussed first. The integration of the component models into a system model for the device and the application of the system model in analyzing the device behaviour will then be presented. In each case, typical examples will be used to highlight the methodology discussed.

The System View of the Device

As discussed before, the entire microfluidic device can be decomposed into a set of discrete components that interact with each other. The analysis of the device

behaviour can then be translated into the analysis of the individual components and of their interaction with each other. This forms the system model of the device (also referred to as the reduced-order or macro model). The system model is a powerful mechanism of describing the system performance. The behaviour of each individual component is inherently stored in the system model. Variations in the behaviour of one component may affect the performance of a second component and the performance of the system as a whole. The system model contains information about the interaction between components and hence enables the analysis of such variations, without requiring the designer to revisit the detailed analyses. The individual components may emerge out of diverse physical domains, as may the designers. The system model thus allows diverse groups to interact with each other in an efficient manner, by defining the information transfer between components in a simple manner.

A typical microfluidic device consists of several discrete systems operating together. These include

- Electrical (voltages and currents)
- Bulk fluid flow (pressure and/or electro-osmotic)
- Mechanical (actuators, membranes)
- Interfaces (capillary breaks, droplets)
- Transport of molecular species in solution (electrophoresis and diffusion)
- Thermal
- Biochemical and electro-chemical
- Optical detection

The electrical system model represents the transport pathways in the device as electrical resistances and inductances, with current and/or voltage sources. Obviously these systems are only meaningful for electrokinetically driven systems

The flow model represents the transport of the bulk carrier (buffer) in the chip. Typical transport mechanisms include electroosmotic, pressure-driven or pneumatically driven flows. The channels on the chip therefore represent resistances to the flow of the bulk fluid. The flow model enables the dynamic analysis of the flow through the device. The flow model is analogous to the electrical circuit model described above.

The mechanical models often serve as the actuation components in the device. For example in an inkjet, the mechanical components may be membranes driven to generate the fluid displacement required to create and eject the droplet.

The interface models contain information about the behaviour of liquid/gas interfaces that exist in the device. These may be menisci and subsequent droplets as in inkjets, or capillary breaks as in several on-chip devices.

The transport model on the other hand describes the motion of the sample through the device. The sample may move along with the bulk or independent of it. The transport model then describes the combined effect of all the transport mechanisms present on the sample location and form.

The thermal model describes the response of the system to temperature changes. Temperature changes may arise because of heating or cooling of the sample in reaction chambers or from the passage of current through the system.

The biochemical and electrochemical models describe the chemistry in the system. These models represent the production and destruction of species in the component. The chemistry in typical devices is often very complex – as a result accurate chemistry models require considerable interaction with experiment in their extraction.

The optical models describe the detection components in the device, especially common in µTAS (Micro-Total Analysis System) based devices [1-5].

The extraction of these models requires detailed analysis of the particular component – specifically its response to various parameters that affect its behaviour. The analysis need not be based on detailed simulation – often, good theoretical analyses are sufficient for practical design purposes. The extracted behaviour then represents the reduced-order behaviour of the device.

An effective tool should provide the designer with the models required to design the device. It should also provide the capability to extend and enhance the models and tailor them to the behaviour of the designer's specific components Finally the design tool should be capable of simulating the extracted system model to characterize the entire device.

In our group we have been involved in developing a tool that meets these requirements. The tool, FlumeCAD, is an integrated design environment consisting of 3D design, modeling and simulation software tools, which enable the creation and analysis of complex microfluidic devices. Inherent in the design flow implemented in FlumeCAD is the ability to translate from a layout of the device to a solid model and to continue to a 3D device model allowing simulations that characterize the various physical phenomena present in the device. This parametrization

can then be represented in a system model and simulated in the FlumeCAD environment.

Examples

In this section we will present examples demonstrating the application of reduced order modeling in the analysis of typical devices. Two cases will be presented – the first an injector/separation column typical of biochip applications and the second an electrostatically driven inkjet. The models presented here are based either on detailed numerical analyses or, in some cases, on theoretical analyses.

Electrokinetic Chip: A typical electrokinetic chip is shown in Figure 1. It consists of ports through which reagents and the sample enter, a reaction site followed by an injection site leading to a separation column. The entire system is driven by electrophoresis. The electrical system model for the device is shown in Figure 2. Each individual channel on the chip is represented by an electrical resistance and inertance. The voltage or current sources are applied at the ports. The system model can be executed in the time-domain by specifying the voltage or current in the sources and the rise time for the specific source. The charge-up time for the field in various components in the system can be determined by this time-domain simulation. This is important in μTAS applications since the field strengths are typically fairly high. A system that charges up slowly is prone to leakage at the intersections by diffusion of the sample – which is generally avoidable.

A second advantage of the electrical system model is in the extraction of boundary conditions for detailed simulations. In general detailed analyses of electrophoresis are conducted at the component level – the currents entering and exiting the domain are dependent on the entire device. These can therefore be easily extracted at the system level and assigned to the appropriate ports for the detailed analyses.

An example of the detailed analysis is described here. The component analyzed is the switched injector, formed by the intersection of two channels. Such intersections are surprisingly powerful tools that enable the definition of sample plugs at the picoliter level [2]; this in turn allows microfabricated electrokinetic systems to outperform their conventional counterparts by orders of magnitude [3].

The number of parameters involved in defining a given injection is large: the currents involved in each step; the length of each step; and the exact geometry of the intersection. It is difficult to explore this entire universe experimentally to optimize the desired properties, and computer modeling of the injection process is thus very useful.

Results from the detailed simulations showing the sample transport and injection are shown in Figure 3. The results have been compared with experiment in [8] and show reasonably good agreement. The experimental conditions are also discussed in [8].

Design analyses of this component can be conducted using the numerical tools. The design analyses analyze the behaviour of the component in response to various parameters that are significant in the design. The behaviour of the injector is generally characterized by the band width of the sample in the separation column that is observed experimentally. The band width is computed from an appropriate model for the optical detection system for the separation column. In a typical system the detector is a point probe, such as a diode or photo-multiplier tube, positioned over the specific location to collect the fluorescence of the species migrating past. In the design tool, the optical model is encapsulated into a Region of Interest (ROI) integrator, which integrates the concentration of species in the specified detection region at any instant in time. The integration can be further correlated to a gaussian to further capture the experimental detection optics.

Examples of the analysis are shown in Figures 4-5. The first example is the effect of the switching field strength on the band width in the intersection. The switching field strength affects the flow in two ways – first, in the width of the plug injected into the separation channel, and second, in the residence time of the plug in the intersection. As discussed before, the plug width is an important quality to define the injection – the residence time, on the other hand, defines the cycle time for the injection – that is, the time between subsequent injections. The dependence of the band width as a function of current in the separation channel is extracted from the design tool by a sequence of simulations, varying the switching current, and performing an ROI integration over the region shown in Figure. The volume of the injected band can also be computed as the integral under the curves and is also shown in the figure on the secondary axis. The band width drops as a function of increasing current, as expected. As the switching current increases further, the injected band width appears to asymptote to a minimum value.

A second issue is the residence time of the species in the intersection. In several applications such as dispensing, the electrokinetic switch is used in a continuous cycle. The cycle time is then dependent on the residence time, since a new fill cycle can only begin well after the previous switch cycle is completed. An ROI integration over the intersection region yields the required residence time as shown in Figure 5, and

therefore indicates an appropriate cycle time as a function of the switching field.

Curves such as those in Figures 4-5 allow the detailed characterization of the flow physics in the injection region. This characterization can then be extended into the system model for the injector and incorporated into a transport model. The system model for the injector can then be coupled to a system model for a capillary separation column. The simplest model for separation only accounts for the advection and diffusion of the species in straight columns. The coupled injector/capillary model is shown in Figure 6. The samples of varying mobility and diffusion constants are driven from the injector into the capillary where they separate. The separation can be detected by coupling a fluorescence detector model at specific points downstream of the injector. The resulting separation is shown in Figure 6 as well. The entire analysis requires minimal simulation time for the transient solution at the reduced-order level. It therefore presents a powerful mechanism to analyze and design these devices.

Inkjet: Inkjet heads are possibly the single most commercially successful MEMS component. In general, an inkjet consists of a source of ink, an actuation mechanism to create the required pressure head to create a droplet and induce the instability required to break off the droplet and a nozzle where the droplet is created and ejected. The system view of the inkjet therefore consists of four major components – the reservoir, the actuator, the main chamber and the nozzle with the meniscus and droplet. These components are connected by appropriate interconnects. Models for these components can be theoretical as well as extracted. In general, the best approach is to start with the theoretical model and refine it based on detailed simulations over the parameter space of significant. An example system model of an inkjet is shown in Figure 7. The individual components in the model are clearly indicated in the figure. The reservoir model is simply a source of pressure in the system. The actuator model generates a flow through the displacement of a membrane that is driven electrostatically. The meniscus/droplet model defines a maximum sustainable droplet size beyond which instability develops causing the droplet to pinch off.

Results from the simulation are shown in Figure 8. The applied voltage on the membrane causes it to deflect and eject a droplet. The resulting meniscus oscillations and their effect on the membrane can also be seen in the figure after the droplet has ejected. The simulation in this case proceeds over four pulses ejecting droplets in each case. The system model allows the user to vary a large number of quantities (geometrical, material and operational) and observe the system behaviour in each case. As before this simulation is also very rapid and the parameter space can be explored rather quickly in comparison to detailed modeling. As a result, it serves as a very effective tool for designers.

Conclusions

Microfluidic systems have generated considerable interest in the past several years. The design of these devices is a complicated process, because of the complex relationships between the device geometry, the properties of the fluids and the operating conditions. The design of these devices is often a trial-and-error process – and is therefore often rather expensive. CAD tools have emerged in the past few years to assist in the design of these devices. Current generation tools provide the capability of performing detailed analysis of the physical processes in these devices. The ability to couple the individual components and their physics into a model enabling the design of the entire device is, as yet, lacking.

A better approach is through the use of reduced-order modeling to create a system-level model for the device. Here the behaviour of each component in the system is captured in a model – these models can then be coupled to analyze the entire system. In our group, we have undertaken the development of FlumeCAD, which is an integrated design tool for this purpose. FlumeCAD allows the detailed analysis of the individual components, provides the capability to extract the behavioural model for the component and enables the incorporation of the extracted model into the system model for the device. Several discrete systems may exist within one device – electrical, transport, flow, optical etc. FlumeCAD aims at enabling the design of devices with one or many such discrete components coupled together in the device.

The current status of FlumeCAD is presented in this paper through two specific examples – the first, an electrokinetic chip – an electrical, transport and optical detection device and the second an inkjet. The examples serve to demonstrate the capability of the tool and of the system modelling concept in generating greater understanding of the device and providing efficient tools in enabling the design of the device.

Acknowledgements

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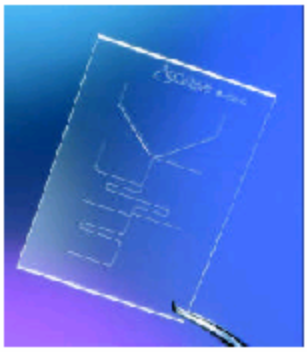

Figure 1: On-chip analysis system showing network of interconnected channels etched in the substrate. The intersections of the channels form the injection locations.

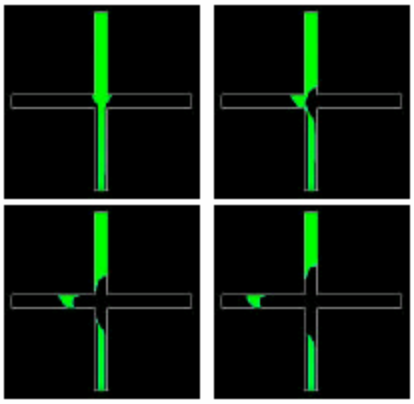

Figure 3: Electrophoretic switching in a cross injector. The flow is first pinched in the intersection and then switched into separation column.

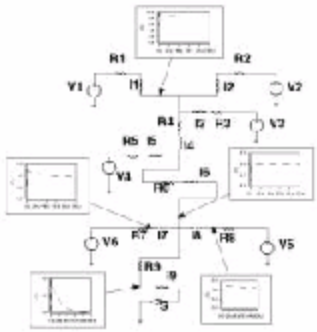

Figure 2: Electrical system model for chip in Figure 1. Ports have Current sources with specified rise time.

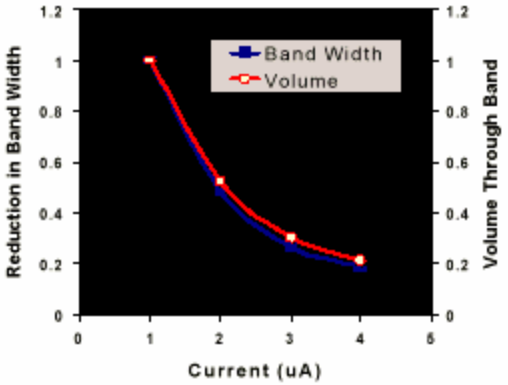

Figure 4: Reduction in Injected Band Width as a function of Field Strength for Electrokinetic Switch.

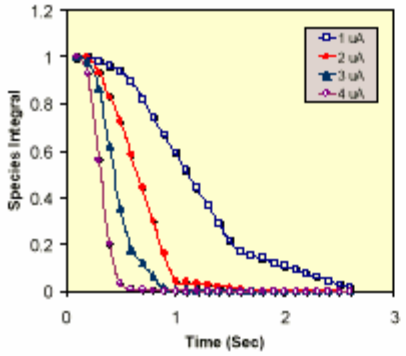

Figure 5: Residence Time of Analyte in Intersection as a function of Switching Current.

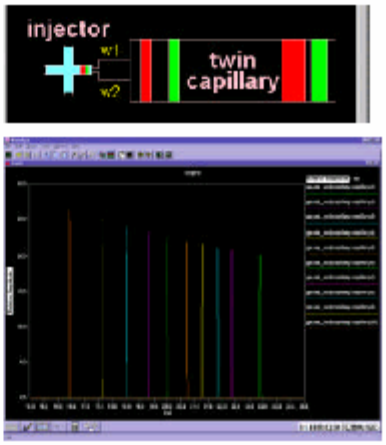

Figure 6: Schematic of Injector/Capillary System model and Results showing electrophoretic separation of 10 samples in a column.

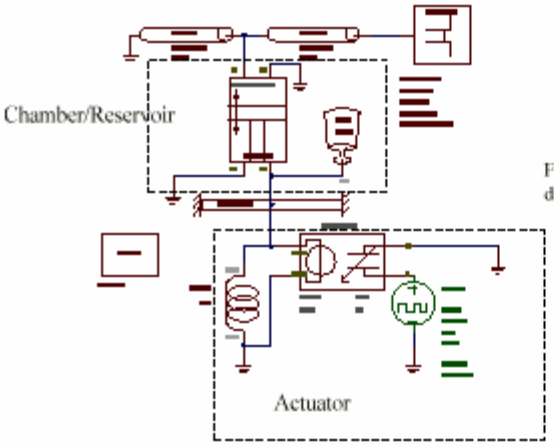

Figure 7: Schematic for electrostatic membrane driven inkjet.

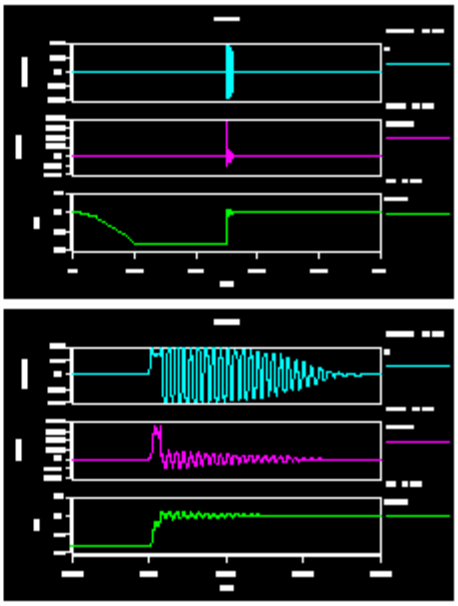

Figure 8: System simulation for inkjet. Top image shows full time sequence and lower image shows a close up of the droplet ejection. In both figures, the top graph is the pressure at the meniscus, the middle is the meniscus location and the bottom the position of the driving membrane.